Operational Atmospheric Chemistry Monitoring Missions

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CAPACITY

Composition of the Atmosphere: Progress to Applications in the user CommunITY

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Capacity Final Report

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Executive Summary

The overall aim of the CAPACITY ('Composition of the Atmosphere: Progress to Applications in the user CommuITY') study has been to define satellite components of a future operational system to monitor atmospheric composition for implementation by ESA/EU within the Space Component of GMES. In this context, *operational* means that: based on the existing, planned and newly-defined missions, a reliable and timely (including near real-time) service of products can be established that will satisfy user needs. *Monitoring* means that: long-term continuity and consistency in the quality of the products can be achieved. *Atmospheric composition* refers to trace gases and aerosols in the atmosphere, and related geophysical parameters such as emissions and surface UV radiation.

In CAPACITY, the missing observational capabilities for an envisioned future integrated system to monitor atmospheric composition have been identified and the space elements needed to remedy these deficiencies have been defined. The principal time frame of the future operational system is projected to cover the period 2010 to 2020 concurrent with the EUMETSAT Polar System MetOp, MSG and MTG and other non-European meteorological operational systems, including NPOESS. In addition, some general recommendations have been formulated for the space elements of a post-EPS operational atmospheric composition system (>2020).

The study team has been able to define the chief implementation strategies for both LEO and GEO mission options, as well as to arrive at further recommendations for the future development of the operational system. Complementarities between mission objectives, instrument capabilities and mission concepts have been exploited wherever possible to provide streamlined options which can deliver effective services.

Study Objectives and Study Team

The CAPACITY study objectives were to:

- identify user applications which would benefit from an operational mission to monitor atmospheric composition, and quantify the user requirements per application;
- derive geophysical data requirements (satellite-borne, ground-based/in-situ, and auxiliary data) for each user application;
- assess the contributions of existing and planned space missions and ground networks to the fulfilment of the geophysical data requirements;
- develop new space segment concepts that could address the identified discrepancies between operational requirements and the capabilities of existing and planned satellite and ground systems;
- define instrument and mission concepts and requirements to address the identified discrepancies from GEO and LEO orbit perspectives, respectively
- evaluate the proposed instrument/mission concepts to identify potentially critical space segment issues;
- evaluate the proposed instrument/mission concepts to identify potentially critical ground segment issues in comparison with the existing baseline concept for a GMES ground segment;

In order to address these objectives a large European consortium has been formed consisting of approximately 30 partners from 9 ESA countries (F, D, UK, I, SW, N, DK, B, NL). The core project team consisted of 4 scientific institutes and 2 industrial partners. The full consortium (Annex A) included a large group of representatives of user organisations, atmospheric scientists using satellite data in combination with models, space research institutes with core expertise in the retrieval, calibration and validation of satellite data, as well as industry with experience in the space and ground segments.

A dedicated User Consultation Workshop was held on 20th/21st January 2004 at ESTEC, soon after the project kicked off in October 2003. A User Feedback Meeting was held on 31 August 2004 in conjunction with the Mid-Term Review. Data users and external experts in atmospheric remote sensing were invited to the final presentation of the study on 2nd of June 2005.

User requirements

The role of representatives of user organizations / communities was considered vital to the study. Users have been active participants in the study as consultants and several users attended the user consultation workshop, user feedback meeting and/or the final presentation.

There has been a strong overlap and continuous interaction with several activities related to operational systems by EU and ESA within the GMES Initial Period and follow-on activities. Relevant projects include GMES-GATO, Daedalus, GEMS, and the ESA GSE Service Element Atmosphere PROMOTE. The user-consultation workshop was organized together with GMES-GATO, with contributions from the aerosol user community via Daedalus. After the workshop several invited organizations became actively involved within PROMOTE.

The potential mission objectives have been organized into three themes, which need to be supported through operational monitoring of atmospheric composition:

(A) Stratospheric Ozone and Surface UV radiation
(B) Air Quality
(C) Climate

For each of the three identified themes three user categories have been identified:

(1) Protocol monitoring,
(2) Near-real time data use
(3) Assessment

Protocol monitoring includes policy support for verification of protocols, legislation and international treaties. *Near-real time data use* includes both forecasting and monitoring by operational (meteorological) centres. *Assessment* includes scientific assessments of long-term environmental threats and associated policy support. The three themes and three user categories result in a total of nine applications which have been designated A1 to C3, e.g., 'A1' refers to the protocol monitoring related to Stratospheric Ozone and Surface UV Radiation,'C3' refers to the assessment of Climate. For each application, the envisaged service to the end users and its quality attributes has been described, together with the expected societal benefits. The services have been translated into requirements on atmospheric composition data and auxiliary data including e.g. meteorological data and bottom-up emission inventories. The user requirements include as much as possible basic information on the geographical and temporal range and resolution of the data, as well as on other relevant quality attributes including accuracy, reliability, stability, delivery time, etc. User requirements are shortly summarized per theme and user category.

For **Stratospheric Ozone and Surface UV radiation** the *protocol* monitoring user requirements stem from the United Nations Montreal Protocol and its subsequent amendments that regulate the release of ozone depleting substances into the atmosphere. The future evolution of the ozone layer needs to be monitored over a period of decades. Also, the UV radiation incident at the earth surface needs to be monitored together with information on ozone, aerosols, clouds and surface albedo. Episodes of high UV exposure, dangerous to man, require a forecast system that relies on *Near Real Time* (NRT) delivery of ozone and some other observations. For scientific *assessment* of the ozone layer recovery and in relation to chemistry-climate interactions a broad range of measurements is required, including ozone depleting substances, polar stratospheric clouds and key species in the catalytic ozone destruction cycles. Vertical resolutions of 2 km or better are required in the upper troposphere and lower stratosphere.

User requirements for **Air Quality** *protocol* monitoring are derived from the EC air pollution directives and the UN ECE Convention on Long Range Trans-boundary Air Pollution (CLRTAP). These include the measurement of ground level amounts of aerosols and gases at city (or higher) scale resolution. For aerosol the demand is for data on particulate matter (PM) at increasingly fine scale, ranging from 10 micron to 2.5 micron and possibly sub-micron size in future. For gases the interest is in ozone, nitrogen dioxide, carbon monoxide, and sulphur dioxide. In order to achieve representative sampling and as a result of the short-term variations of the sources and sinks of these species near the surface, high temporal sampling of 1-2 hours is needed during daytime. The need to make accurate forecasts of air quality for health and regulatory reasons requires *Near Real Time* delivery of a similar set of observations, with again a high temporal and spatial sampling frequency during daytime and night time measurements being desirable. For air quality *assessment* and its long term evolution, the oxidising capacity of the atmosphere is the main driver of the observational requirements. Here, the hydroxyl radical OH plays a pivoting role that needs to be constrained by measurement of key species in the troposphere on a global scale.

Climate *protocol* monitoring requirements have been derived from the Kyoto Protocol and concern the emissions of greenhouse gases carbon dioxide, methane, nitrous oxide, and some minority gases. Anticipating on future needs, also tropospheric ozone and aerosol are included in these requirements as well as the tropospheric ozone precursor gases carbon monoxide and nitrogen dioxide. The observational requirements for climate gases arise from the need to improve our knowledge on anthropogenic and biogenic sources and sinks and specifically to narrow down the uncertainties in emission inventories. Climate monitoring and numerical weather prediction by operational centres require *Near Real Time* availability of several climate relevant gases and aerosols for assimilation. For climate *assessment* the driver for the requirements is the need to understand climate-chemistry interactions, including radiative, dynamical and chemical processes and feedbacks and their response to global climate change. The requirements include the measurement of water vapour and ozone at 2 km vertical resolution.

Geophysical data requirements per application area

For each of the nine application areas a comprehensive set of measurable geophysical quantities has been compiled, directly traceable to the user requirements. Per application area a measurement strategy has been formulated to define how to optimally construct an integrated end-to-end system that is based on three complementary building blocks:

- Satellite data products,
- Ground-based and in-situ observations
- Auxiliary data, including meteorological data and emission inventories

Separate data requirement tables have been constructed for the satellite data products (in terms of level-2 products, here defined as retrieved geophysical data products) and for the ground-based / in-situ observations. Therefore, a total of eighteen tables have been compiled for the nine applications.
Per theme and user category the most relevant data products and processes (physical, chemical) have been identified and discussed. Drivers have been specified for each of the data product. Typical drivers include, e.g., forecasting, concentration monitoring, emission monitoring, trend monitoring, and validation (for ground-based / in-situ observations). For the assessment drivers include also fundamental processes such as ozone loss and ozone recovery and composition-climate interactions including radiative forcing, the oxidising capacity and the Brewer-Dobson circulation. For each compound height-resolved and height-integrated products have been distinguished. Per product the relevant height range, horizontal sampling and vertical resolution, revisit time and uncertainty have been quantified, based on expert judgments by scientists including atmospheric chemistry modellers. The variability of the compound in the atmosphere has been found to be one useful measure, as well as the typical temporal and spatial scales of the driving processes that lead to the observed variability.

Near real time data delivery for the different applications typically imply that the data needs to be available to an operational modelling environment within a couple of hours after observation. In that case a significant part of today's observations can still be used for the analysis on which forecasts for tomorrow (etc.) can be accurately based.

In the compilation of the quantitative data requirements extensive reference has been made to several activities that have been undertaken earlier to formulate requirements for observing atmospheric composition: the WMO/CEOS report on a strategy for integrating satellite and ground-based observations of ozone; the IGOS "Integrated Global Atmospheric Chemistry Observations" (IGACO) report; the WCRP/SPARC defined observational requirements for long-term scientific observations; the EUMETSAT nowcasting requirements in Golding et al.; the user requirements from the Eumetsat MTG preparation activities; and observational requirements defined for atmospheric chemistry research missions proposed in the frame of ESA's Explorer programme (ACECHEM, GeoTROPE).

Assessment of existing and planned satellite missions and ground networks

The ground network, current satellite missions and new satellite missions planned for 2010-2020 were reviewed to evaluate their contributions to monitoring of atmospheric composition. Particular attention was paid to the operational observing system in polar orbit constituted by MetOp and NPOESS. This included a quantitative comparison of sensor performance against geophysical data requirements for each application based on the best information available to the study team for each sensor. For the ground network and current satellite missions, demonstrated sensor performances were used, whereas for future satellite missions they were estimated from contemporary missions and retrieval simulations supplied to the study team from other projects. The review confirmed that the ground networks and satellite missions planned for 2010-2020 would make valuable contributions to atmospheric composition monitoring in that period. However, the review also identified a number of limitations which can be summarised as follows:

- Spatio-temporal sampling of the boundary layer by MetOp and NPOESS is too sparse to comply with the stringent requirements for air quality applications. Their sampling of the boundary layer is limited by two factors: (a) ground-pixel size, which determines how frequently observations can be made between clouds and (b) equator crossing times. In particular, observations of O_3 and short-lived pollutants such as NO_2, H_2CO and SO_2 will be made at ~9:30am by GOME-2 and ~1:30pm by OMPS but not later in the day, as needed for attribution of afternoon pollution episodes and for early morning forecasts of air quality.
- Spectral coverage extending to wavelengths longer than GOME-2 and OMPS is needed to measure CH_4 (and CO) in the boundary layer and to resolve tropospheric aerosol into different layers, as needed for climate and air quality applications. Additional channels would be needed in the Short-Wave Infra-Red (SWIR) near 2.0 μm and 2.3 μm.
- To target tropospheric trace gases (e.g. non-methane hydrocarbons) additional to those measured by IASI and CrIS, a nadir mid-infrared (MIR) instrument with higher spectral resolution would be needed, i.e. similar to TES.
- Requirements for sounding trace gases and aerosol in the upper troposphere and stratosphere will not be addressed by MetOP or NPOESS, with the exception of stratospheric O_3 (GOME-2 & OMPS) and stratospheric aerosol (OMPS). These requirements are currently being addressed by the Odin, Envisat and Aura limb-sounders, but none of these are likely to still be functioning beyond 2010.
- No UV-VIS or IR solar occultation sensors for long-term monitoring of stratospheric trace gas and aerosol profiles are currently planned after MAESTRO and ACE on SCISAT, which are unlikely to still be functioning beyond 2010.
- The vertical resolution of ground based sensors is not sufficient in a number of cases to meet requirements placed on them for height-resolved measurements.

The following table summarises MetOp/NPOESS main non-compliances with respect to the spaceborne geophysical data requirements per theme and user category. The degree of non-compliance is denoted either as '***major***', i.e., key measurements will not be made in the required height-range and/or time of day, or as '***significant***', i.e., key measurements made by MetOp/NPOESS will seriously non-comply in vertical resolution, horizontal and/or temporal sampling or precision.

Application	User Category		Degree of non-compliance	Notes
Stratospheric Ozone/ Surface UV radiation	Protocol Monitoring	A1S	--	--
	Near-Real Time Use	A2S	Major	1
	Assessment	A3S	Major	1
Air Quality	Protocol Monitoring	B1S	Significant	2
	Near-Real Time Use	B2S	Major	2
	Assessment	B3S	Major	2
Climate	Protocol Monitoring	C1S	Significant	3
	Near-Real Time Use	C2S	Major	1
	Assessment	C3S	Major	1

Table 1 *Degree of MetOp (GOME-2, IASI, AHVRR) / NPOESS (OMPS, APS) non-compliance with respect to spaceborne geophysical data requirements per theme and user category.*

Note 1: Absence of profile data in upper troposphere and stratospheric, except for O_3 , aerosol and NO_2 to be supplied by OMPS-limb.
Note 2: Serious non-compliance on spatio-temporal sampling of the (lower) troposphere. Absence of data later than the 1:30pm OMPS measurement will compromise detection and attribution of pollution episodes occurring in the afternoon and impact on Air Quality forecast. Vertical resolution of height-integrated measurements is dependent on assimilation into atmospheric models.
Note 3: Lack of boundary layer sensitivity for CO, CH_4 and CO_2 and aerosols.

Identification of new satellite components for integration into the operational observing system

The contributions of the planned operational missions and ground-based networks towards any of the established applications have been identified. In the next step, the discrepancies between the capabilities of the existing and planned missions and the geophysical data requirements were considered. It is concluded that with respect to the space segment of a measuring system for operational monitoring in the 2010-2020 time period there are three overall requirements that cannot be met by the planned systems:

- High temporal and spatial resolution space-based measurements of tropospheric composition including the planetary boundary layer (PBL) for Air Quality applications (B1, B2, B3)
- High vertical resolution measurements in the upper troposphere/lower stratosphere region for Stratospheric Ozone/Surface UV and Climate near-real time and assessment applications (A2, A3, C2, C3)
- High spatial resolution and high precision monitoring of tropospheric climate gases (CH_4, CO and CO_2) and aerosols with sensitivity to boundary layer concentrations (C1)

Space system concepts were developed to provide the necessary enhancements to current monitoring capacity through adaptation and re-flight of proven instruments or implementation of well developed generic instrument types. The analysis recognised the variety of instrument types that can contribute to the information requirements and hence a "hierarchy of capability" approach was adopted illustrating the improvement of performance from minimum specification to maximum specification. Thresholds for "significant Capacity capability" for operational missions were identified as well as priority instrument performances.

For the ***Stratospheric Ozone/Surface UV*** theme it was concluded that only the A1 theme requirements can be met by the planned MetOp and ground-based systems. The other stratospheric A2 and A3 themes require limb sounding capabilities. For A2, only ozone profiles are mandatory but measurements of other species are highly desirable: ClO, polar stratospheric clouds, stratospheric aerosol, HNO_3, H_2O, tracers, and HCl. For A3, all the A2 measurements are required with, in addition, HCFCs, $ClONO_2$, and SO_2 (enhanced). A limb MIR system is therefore suggested although limb MM also has significant capabilities, particularly in cloudy regions of the atmosphere. A limb UV-VIS instrument can monitor the important compounds of NO_2 and BrO.

For ***Air Quality***, it was shown all systems (B1 to B3) were essentially similar with a prime requirement for high spatial (<20 km) and temporal (<2 hours) resolution measurements of O_3, CO, NO_2, SO_2, HCHO, and H_2O (B2/B3), with sensitivity to the PBL. Instruments are likely to be nadir UV-VIS-NIR with either Short-Wave Infra-Red (SWIR) or Mid Infra-Red (MIR) capability for CO. For B3 particularly, aerosol measurements at multiple wavelengths would enhance the system ideally in conjunction with night-time measurements.

For ***Climate***, the C1 protocol monitoring system was notably different to those for C2 and C3. Kyoto protocol monitoring demands high precision measurements of CH_4 and CO (and CO_2) building on the SWIR measurements demonstrated by SCIAMACHY. Improved NO_2 measurements (spatial resolution of 10 km) would also be ideal. It is suggested that C1 systems could be combined with B1 to B3 systems in the evolution of the GMES system. For C2 and C3, the priorities are limb sounder measurements for high vertical resolution (<2 km). For C2, measurements of H_2O, O_3, CH_4, and N_2O suggest either limb MM or limb MIR whereas for C3, limb MIR is more likely to be a priority to measure the large range of necessary species to monitor changes in radiative forcing, oxidising capacity and stratospheric ozone with sensitivity also to the upper troposphere.

Definition of GEO Instrument / Mission Concepts and Requirements

The derivation of mission and instrument requirements for the geostationary orbit (GEO) component of an operational atmospheric chemistry mission has been driven by the Air Quality user need to have a revisit time less than two hours in combination with a high horizontal resolution and frequent cloud free sampling of the lowest part of the troposphere. The relevant user services are requesting data for Europe and surrounding areas.

The frequency of cloud free sampling was quantified within this study. It was assessed how many cloud free observations per day and per geo-location are typically available from geostationary orbit, depending on the instrument field-of-view. Based on MVIRI/METEOSAT cloud statistics it is concluded that an instrument in GEO orbit with 5×5 km^2 at sub-satellite point (SSP) will deliver over Europe on average ~5 (~2 in winter to ~8 in summer) cloud free observations per day per geo-location. With 15×15 km^2 (at SSP) it will deliver on average ~3.5 (1.5 in winter to ~6.5 in summer) cloud free observations. In comparison, the planned METOP and NPOESS instruments in LEO do not allow for daily cloud free observations and have much reduced spatial density.

The instrument types and spectral ranges that have been identified suitable to satisfy the satellite data requirements (Level 2) by adding a geostationary component include:

- A solar backscatter nadir sounding instrument covering Europe and surrounding areas to provide total and tropospheric columns of O_3, NO_2, SO_2, HCHO, H_2O and CO, as well as aerosol optical thickness during day time, including the lowest troposphere, at one hour temporal sampling and at 5×5 km^2 (at SSP) horizontal resolution, fulfilling day time Air Quality user requirements with the exception of improved vertical sampling in the troposphere.
- A thermal IR sounder (15×15 km^2 (at SSP); one hour temporal sampling) adapted for a combined solar backscatter and thermal IR sounding mission covering Europe and surrounding areas to provide O_3 and CO with vertical resolution in the troposphere. The IR sounder also provides night-time coverage of O_3 and CO and some additional species: PAN, N_2O_5, and HNO_3.

Requirements on instrument level (radiometric, spectral and geometric) have been formulated to match as close as possible the level-2 geophysical data requirements and some specific mission requirements have been added. The performance of the specified instruments with respect to level-2 data requirements was determined by analogy of already proven instrument concepts in LEO and their validated level-2 products as well as by reviewing previous sensitivity studies and performing a few new retrieval simulations. It was concluded, that the majority of the user requirements can be met, especially with respect to the demanding horizontal resolution and temporal sampling requirements.

Definition of LEO Instrument / Mission Concepts and Requirements

Measurement techniques were reviewed to identify the contributions which each could potentially make to monitoring atmospheric composition from low earth orbit (LEO), focusing specifically on the value which each would add to the planned operational observing system constituted by MetOp/NPOESS. To inform this review, quantitative comparisons against observational requirements were performed for each application using performance estimates from retrieval simulations for instrument specifications, which were made available to the study from other projects. Findings were then drawn for each application in regard to the overall value, which each measurement technique could add to the planned operational system. In principle, this system could be augmented in three physical dimensions:

Geometrical Deployment of a nadir-viewing UV-VIS-NIR spectrometer with ground pixel significant smaller than GOME-2/MetOp and OMPS/NPOESS would increase the density of observations of the boundary layer ~30 times going from 80×40 km^2 (GOME-2 nominal mode) to 10×10 km^2 pixels and, simultaneously, it would about triple the chance per pixel for a cloud-free scene. Secondly, the operational system is devoid of limb-viewing emission sounders to provide height-resolved global data in the upper troposphere and stratosphere for *operational users* and solar occultation sensors to extend stratospheric vertical profiling by this established technique for use in *scientific assessments*.

Spectral The operational system does not cover the wavelength range 0.8 – 3.7 µm. The addition of two channels near 2 µm (SWIR) to the nadir-viewing UV-VIS-NIR spectrometer would (a) increase sensitivity to CH_4 and CO in the boundary layer and (b) resolve aerosol into tropospheric layers, which would add significantly to the operational system for *climate* applications. Secondly, the deployment of a nadir MIR instrument with spectral resolution higher than IASI/MetOp and CrIS/NPOESS would provide data of higher quality on CO and enable detection of non-methane hydrocarbons. Thirdly, deployment of a limb-UV-VIS-NIR sounder with (a) higher spectral resolution in BrO and NO_2 bands and (b) channels added in the 1 – 2µm (SWIR) range would improve compliance of the operational system for Stratospheric Ozone / Surface UV and Climate *scientific assessments*.

Temporal Afternoon observations of trace gas pollutants in the boundary layer would be unique for polar orbit, allowing pollution episodes in the afternoon to be attributed and more timely observations than GOME-2/MetOp at 9:30am or OMPS /NPOESS at 1:30pm for air quality forecast the following morning.

To arrive at final recommendations other criteria that were considered included the priority given to operational users and the instrument maturity and heritage within Europe.

In conclusion, the main recommendation from LEO perspective is, as a first step, to implement a single dedicated Sentinel platform carrying nadir-viewing UV-VIS-NIR-SWIR instrumentation in an afternoon orbit to complement MetOp/NPOESS in 9:30am and 1:30pm daytime equator crossing times, and to better serve the needs of users for operational Air Quality applications and Climate Protocol Monitoring. For post-EPS it is recommended to follow a phased, incremental approach from the MetOp/NPOESS system towards an operational monitoring system, which can optimally serve user needs for atmospheric composition monitoring. Implementation could also benefit from international co-operation, e.g. with respect to a solar occultation mission in which heritages in USA, Canada and Japan are stronger than in Europe.

Initial Evaluation of Proposed Instrument / Mission Concepts to Identify Potentially Critical Space Segment Issues

The instrument and mission requirements for the geostationary (GEO) and low-earth orbit (LEO) components have been reviewed and iterated. None of the assessed concepts is completely new; similarities to existing investigations are shown (MTG, GeoTROPE and ACECHEM). To outline radiometric instrument performance some mathematical simulations have been performed. Some improvements are needed to achieve in LEO a limb mission with higher vertical resolution. In future studies more detailed analyses are needed to show the full technical impact of the required modifications in combination with the predicted technologies. Based on the preliminary conceptual instrument designs resulting budgets for power and mass are established and compared. The budgets give a qualitative indication for the needed development effort of the different instrument designs. It is expected that further iterations on instrument requirements may change the preliminary conclusions. Nevertheless the UV-VIS-NIR-SWIR instrument concept required for both GEO and LEO probably needs the lowest development effort combined with the highest heritage.

An additional assessment is performed on mission design alternatives to the conventional GEO and LEO options. Given requirements on mission reliability for an operational mission a constellation of three satellites in low-earth orbits is an interesting compromise with cost advantages, especially if the same set of instruments can be used. Revisit time requirements of 0.5 to 2 hours as required for Air Quality applications are not fulfilled by a sun-synchronous three-satellite constellation. A reasonable rise of the orbit altitude is undesirable for an operational mission because the impact of protons radiation on satellite and instrument design, lifetime and costs is increasing with altitude. However, with lower inclinations a revisit time below 2 hours is feasible for 894 km orbit altitude. Because this orbit has not yet been used for earth observation applications in Europe, it is recommended to study such a constellation in detail taking all measurement and technical aspects into account. The changing local time of the spacecraft will have strong impact on the evaluation of the observations, power and thermal spacecraft system.

In conclusion, the GEO mission and LEO mission requirements are complementary. A combined mission based on a constellation of three satellites in an orbit with low inclination may be a compromise for future systems. More detailed trade-off analyses of potential implementation scenarios are recommended to balance the needed development effort against the observational performance and the priority of the different mission objectives.

Initial Evaluation of Proposed Instrument / Mission Concepts to Identify Potentially Critical Ground Segment Issues

The architecture and key features of the ground segment for future atmospheric chemistry monitoring missions has been outlined. General ground segment requirements for the envisioned user services have been identified. Similarities and differences with the available GMES ground segment concepts have been identified. The main conclusions from the general evaluation include that the ground segment for the proposed LEO and GEO missions is feasible and that no show-stops have been identified. However the main issues are how to integrate the existing models (distributed ground segment over Europe) and what are the end-to-end timeline for product distribution versus the specification (0.5 to 2 hours for Air Quality monitoring). Nevertheless, specific care has to be paid to the development of operational autonomous modelling and processing capabilities, as well as to the receiving stations required for near-real time product delivery from the LEO mission, possibly overcrowded by the suite of GMES space missions.

In future studies more detailed and quantified analyses will be needed on the definition of the products at different levels and on the required processing facilities, as well as on the operational status of the envisioned models for the user services. In these studies the different levels of processing shall be clearly identified and distinguished.

Overall Conclusions

In this study, CAPACITY, requirements for future atmospheric chemistry monitoring missions have been defined. The study findings support an integrated and international approach to operational monitoring of atmospheric composition to which space missions, ground-based and in-situ observations and modelling information all contribute. This overall concept is inline with the IGACO recommendations.

The complete chain from user requirements via geophysical data requirements to instrument, mission and ground segment requirements has been identified, starting from the foundation provided by the operational observing system planned for 2010-2020 (satellite and ground network) in Europe and internationally.

Candidate operational missions were evaluated taking into account the following criteria:

- The user need for operational services and urgency of the envisioned applications
- The added value over existing and planned operational systems and space elements
- The maturity of the mission concept for operational implementation

Three specific requirements for satellite observations that cannot be met by the planned operational systems have been highlighted and these include specifically a sufficient spatio-temporal sampling for the Air Quality applications, high vertical resolution measurements in the upper troposphere and lower stratosphere for the Stratospheric Ozone/Surface UV and Climate near-real time and assessment applications and measurements of climate gases (CH_4, CO, CO_2) and aerosols with sensitivity into the planetary boundary layer for Climate Protocol Monitoring.

Below we summarise the study findings per theme and give some recommendations for implementation.

Air Quality

The combination of requirements on revisit time, resolution and coverage, including frequent cloud-free sampling of the planetary boundary layer, is very stringent. The Air Quality requirements to meet user needs are not adequately addressed by the planned operational missions. Planned operational missions in LEO will contribute to, but by and large do not fulfil stringent Air Quality sampling requirements. Nominal mission lifetimes of the Envisat and EOS-Aura missions both end before 2010. Continuation of Air Quality user services based on these missions requires quick action to be taken. Moreover, planned operational missions have primarily meteorological and climate objectives. The Air Quality applications could benefit most from denser spatio-temporal sampling over Europe for forecasting and monitoring as well as globally for worldwide Air Quality monitoring and attribution of pollution episodes. The Air Quality user requirements include a suite of trace gases as well as aerosols.

CAPACITY concludes on the Air Quality theme:

- that the monitoring for operational Air Quality applications needs to be optimised with respect to the density of spatio-temporal sampling of the planetary boundary layer,
- that small ground pixels are needed to maximize (cloud-free) sampling of the boundary layer,
- that it is important to cover diurnal variations for Air Quality
- that regional coverage with short revisit time is needed to optimally serve regional Air Quality forecasting and monitoring in Europe and that global coverage is required for the monitoring and assessment of Air Quality, the oxidising capacity, and the quantification of continental in/outflow.
- that *afternoon* observations would complement best the observation times of day of MetOp and NPOESS observations in the post-Envisat/post-EOS-Aura time period

For **implementation** of the Air Quality Mission CAPACITY recommends:

- to enhance observational capabilities in the 2010-2020 time period and afterwards for operational Air Quality applications with respect to the density of spatio-temporal sampling of the planetary boundary layer by a combination of space elements in Geostationary Orbit (GEO) and Low-Earth Orbit (LEO). The global (LEO) and regional (GEO) missions are of equal importance.
    - A LEO mission with a UV-VIS-NIR-SWIR nadir viewing spectrometer with ground pixel size significantly smaller than GOME-2 and OMPS and daily global coverage in a polar orbit with *afternoon* equator crossing time optimally chosen to complement on the times of day of MetOp and NPOESS observations in the post-Envisat/post-EOS-Aura time period and to maximize (cloud-free) sampling of the boundary layer. Global coverage is required for the monitoring and assessment of Air Quality, the oxidising capacity, and the quantification of continental in/outflow.
    - A combined GEO mission with a UV-VIS-NIR-SWIR spectrometer and TIR sounder with small ground pixel sizes to cover diurnal variations in O_3, CO, NO_2, SO_2, HCHO, HNO_3, PAN, N_2O_5, organic nitrates and aerosols, height-resolved tropospheric O_3 and CO, and to significantly improve upon the cloud-free sampling of the planetary boundary layer over Europe.
    - Taking into account maturity, cost and risk issues, it is recognised that a LEO mission could have a somewhat shorter lead time, even though it will only partially fulfil the requirements of European Air Quality users.
- to prepare for phase A studies in 2005/2006 for LEO and GEO missions targeting Air Quality (Protocol Monitoring, Forecasting and Assessment) based on the given definitions of the instrument / mission concepts and requirements and their subsequent evaluation, and taking into account the importance of cloud statistics on lower tropospheric observations.

Climate Protocol Monitoring

For the monitoring of greenhouse gas and precursor emissions the planned operational missions fall short in their capabilities to observe CH_4, CO and CO_2 with sensitivity to, and frequent cloud-free sampling of the planetary boundary layer which is required to derive surface emissions. In addition, improved aerosol observations are required.

CAPACITY concludes on the Climate Protocol Monitoring theme:

- that concentration and emission monitoring is needed for O_3, NO_2, SO_2, CO_2, CO, CH_4, and aerosols
- monitoring for operational Climate Protocol applications needs to be optimised with respect to the density of spatio-temporal sampling of the planetary boundary layer,
- that small ground pixels are needed to maximize (cloud-free) sampling of the boundary layer,
- that it is limited important to cover diurnal variations for Climate protocol monitoring
- that global coverage is required, while regional coverage with short revisit time will optimally serve climate protocol monitoring in Europe.

For **implementation** of the Climate Protocol Monitoring Mission CAPACITY recommends:

- that the Air Quality Monitoring Missions (LEO and GEO) be most efficiently extended to include Climate Protocol Monitoring by addition of SWIR channels.
- to extend the phase A studies in 2005/2006 to investigate the added value of the Air Quality missions for Climate Protocol Monitoring based on the given definitions of instrument / mission concepts and requirements and their subsequent evaluation.
- that given the very stringent uncertainty requirements on CO_2 the implementation of operational monitoring of CO_2 for emission monitoring is not recommended until useful capability has been shown by the planned OCO (NASA) and GOSAT (JAXA) research missions.

Climate Monitoring, Climate Assessment and Stratospheric Ozone/Surface UV radiation
Planned operational missions fall short in the monitoring and assessment of composition-climate interactions. Specifically, it is needed to better resolve (long-term changes in) the vertical structure of the atmosphere, especially with respect to ozone and water vapour, which are very important, radiatively (climate forcing), chemically (ozone recovery, oxidizing capacity) and dynamically (Stratosphere-Troposphere connections, Brewer-Dobson circulation).
For stratospheric Ozone/Surface UV radiation planned operational missions fall short in their capability to resolve (long-term changes in) the vertical structure of the atmosphere for several long-lived compounds. Adequate vertical resolution of the order of a few kilometres in the upper troposphere and stratosphere is needed for scientific assessments of the ozone shield and would also allow improvement of the forecasting applications.

CAPACITY concludes on the Climate and Stratospheric Ozone/Surface UV radiation near-real time and assessment applications:

- that planned operational missions contribute significantly to the Protocol Monitoring ('Montreal') and near-real time ozone and UV applications
- that user needs for height-resolved data on O_3, H_2O, and other trace gases and aerosols in the upper troposphere and lower stratosphere can not be met because planned operational missions have only nadir-viewing instruments – with the exception of OMPS, which mainly targets O_3.

For **implementation** of the Climate and Stratospheric Ozone/UV radiation Near-real time and Assessment Applications CAPACITY recommends:

- to move incrementally towards an optimal operational monitoring system for these applications, in line with the GMES overall concept.
- to enhance the observational capabilities in vertical resolution in the 2010-2020 time period for the Climate and Stratospheric Ozone and Surface UV radiation near-real time and assessment applications.
- instrument specifications for limb-MIR and limb-MM techniques – feasible options with complementary capabilities – be consolidated to meet user requirements for a future operational limb-sounding component.
- to prepare for a phase A study in 2005/2006 for a limb sounding component to the LEO mission targeting Climate (Near-Real Time Monitoring and Assessment) and Stratospheric Ozone (Forecasting and Assessment) based on the conclusions drawn in the "Definition of LEO instrument / mission concepts and requirements" and its subsequent evaluation.

Alternative constellations and type of orbits
Finally, for alternative constellations and type of orbits the following general recommendation is made:

- to investigate the possibility, advantages and disadvantages of a constellation of satellites in low inclination orbit to addresses the CAPACITY operational applications in the post-EPS time frame.

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Preface

This study has been run by a core group of four scientific institutes and two industrial partners. However, it is acknowledged that several important contributions to the study have been made by a large group of consultants. Several user organisations and specialists have contributed to the definition of the user requirements and have helped to clarify how atmospheric composition data could be used in operational applications. The following list of user organisations has been involved in the definition of the user requirements.

> Ademe, CNR-ISAC, DLR-IPA, ETH, Eumetnet(via DMI), Eurocontrol, JRC-EIS, Meteo-France, MPI Mainz, NILU, RIVM (ETC-ACC), TNO-FEL, Univ. Heidelberg, WMO

Note that the user organisations in CAPACITY have large overlap with the user organisations that were involved in the preparation of the GSE project 'PROMOTE' at the end of 2004. Furthermore, for CAPACITY a group of scientific institutes has been added to deliver information on the user requirements on long-term science issues.
Scientists running atmospheric-chemistry models have helped extensively in the definition of the measurement strategy and the quantification of the geophysical data requirements per application area. Critical reviews of the user and data requirements have been given by invited experts at the User Feedback Meeting, halfway the project. Retrieval experts from several institutes have given invaluable inputs to the assessment of existing and planned space systems and ground networks, as well as to the definition of the ultimate GEO and LEO mission concepts.

The following people have contributed to the 'Capacity' project, next to the project team members:

User Requirements Len Barrie, Geir Braathen, Bram Bregman, Martin Dameris, Christian Elichegaray, Aasmund Fahre Vik, Jack Fishman, Sandro Fuzzi, Allan Gross, Isabel Jeanne, Robert Koelemeijer, Maarten Krol, Steinar Larsen, Gerrit de Leeuw, Jos Lelieveld, Arthur Lieuwen, Thierry Marbach, Frank McGovern, Peter den Outer, Joseph Pacyna, Thomas Peter, Vincent-H. Peuch, Robert Pierce, Ulrich Platt, Frank Raes, Martin Riese, Daniel Schaub, Jan Schaug Martin Schultz, Jens Sorensen, Henning Staiger, Kjetil Thorseth, Andreas Volz-Thomas, Thomas Wagner, Andrea Weiss, Sabine Wurzler, and participants to the user consultation workshop, 20-21 January 2004, ESTEC, Noordwijk, The Netherlands.	**Geophysical Level 2/3 Data Requirements** Peter Bergamaschi, Gilles Bergametti, Olvier Boucher, Bruno Carli, Hendrik Elbern, Henk Eskes, Jean-Marie Flaud, Michael Gauss, Didier Hauglustaine, Ivar Isaksen, Howard Roscoe **Integrated Observing Systems** Gary Corlett Simon A. Good	**Specification of instrument and mission concepts and requirements for Geostationary Orbit** Gilles Bergametti, John Burrows, Thomas von Clarmann, K.U. Eichmann, Jean-Marie Flaud, F. Friedl-Vallon, Otto Hasekamp, Stefan Noel, Johannes Orphal, V. Rozanov, T. Steck, Gabi Stiller
	Assessment of existing and planned systems and ground networks Ilse Aben, Francois-Marie Bréon, Claude Camy-Peyret, Cathy Clerbaux, Thomas von Clarmann, Jean-Marie Flaud, Herbert Fischer, Victoria Jay, Rienk Jongma, Barry Latter, N. Lautié, Ahilleas Maurellis, Martine de Maziere, Pascal Prunet, Avri Selig, Richard Siddans, Gabi Stiller, Carmen Verdes	**Specification of instrument and mission concepts and requirements for Low-Earth Orbit** Ilse Aben, Francois-Marie Bréon, Claude Camy-Peyret, Cathy Clerbaux, Thomas von Clarmann, Jean-Marie Flaud, Herbert Fischer, Victoria Jay, Rienk Jongma, Barry Latter, N. Lautié, Ahilleas Maurellis, Pascal Prunet, Avri Selig, Richard Siddans, Gabi Stiller, Carmen Verdes

International Context, General Approach and Outline

Relevant Earth Observation programmes and initiatives

International

GEOSS
As a result of the first Earth Observations summit held 31 July 2003 in Washington an inter-governmental *ad hoc* Group on Earth Observations (GEO) was established, tasked with the development of a conceptual framework and a 10-year implementation plan for the building of a comprehensive, coordinated and sustained Global Earth Observation System of Systems (GEOSS).

The group and a number of sub-groups on User Requirements and Outreach [RD5], Architecture, Data Utilisation, Capacity Building and International Cooperation have produced the required plans. At the second EO Summit held in Tokyo 25 April 2004 the framework plan has been adopted. At the third EO summit in Brussels 16 February 2005, organised by the European Union, the GEOSS 10 year implementation plan has been approved. In 2005, governing structure and funding provisions are being established.

The need for better information according to GEO, is driven by the notion that current efforts are fragmented and plagued by (1) lack of access to data in the developing world, (2) eroding technical infra structure, (3) large gaps in spatial and temporal coverage of observations, (4) inadequate data integration, (5) uncertainty in continuity of the observations, (6) inadequate user involvement, (7) lack of processing systems to transform data into useful information.

The GEO pledge is to progress from the separate observation systems and programmes of today, to timely, quality and long-term global information as a basis for future sound decisions and policy-maker action. The GEOSS system proposed will be a distributed system of systems, building on current cooperation efforts and allowing existing observing systems to remain within their mandate whilst encouraging and accommodating new components. The system will be user-driven and data produced by the system will be accessible to users in open and unrestricted way, whilst respecting (inter)-national laws and agreements. A number CAPACITY partners are member of the GEO ad hoc Group.

IGOS-P
The Integrated Global Observing Strategy Partnership (IGOS-P) brings together the efforts of a number of international bodies concerned with the observational component of the Earth System, both from the research and the operational side. The IGOS Partnership was established in 1998 and is aimed at the definition, development and implementation of a global Earth Observation strategy. The main line of thinking in this strategy is to first identify the user needs, then to ascertain how well user requirements are met by existing observation systems and finally, how observations could be improved in future by better integration and optimisation of ground, airborne and space-based observation systems. IGOS works through approved themes, one of them being the Integrated Global Atmospheric Chemistry Observation strategy (IGACO).

IGOS-IGACO
The objective of IGACO [RD1], is to define a feasible strategy for deploying an Integrated Global Atmospheric Chemistry Observation System (IGACO) , by combining ground-based, airborne and satellite observations with suitable data archives and global models. The purpose of the system is to provide representative, reliable and accurate information on the changing atmosphere to those responsible for environmental policy development and to weather and environmental prediction centres. The IGACO strategy will also improve scientific understanding of the changing atmosphere.

The IGACO system includes the following components:

- Networks of ground-based instrumentation to measure ground concentrations and vertical profiles of atmospheric constituents and UV radiation on a regular basis.
- Regular aircraft measurements of chemical and aerosol species in the entire troposphere, and in the upper-troposphere / lower-stratosphere (UTLS) layer, to obtain in-situ vertical profile information.
- Satellite based instruments preferably mounted on a combination of LEO (low-Earth orbit) polar and GEO (Geo-stationary) equatorial orbiting satellite platforms, for obtaining remote sensing data at required spatial and temporal resolution.
- Theoretical models capable of integrating the measurements derived from different sources at different times and locations (data assimilation) and able to assess the quality and consistency of the measurements.

Four main atmospheric chemistry themes have been identified:

- Air Quality: the globalisation of Air Pollution
- Oxidising efficiency: the Atmosphere as a waste processor
- Stratospheric Ozone shield
- Chemistry–Climate interaction

For each of these themes a set of required observables have been identified, specifying spatial and temporal resolution and accuracy. Taking into account financial and logistic constraints a group 1 set of observables has been defined that can be measured by existing or approved observation systems with some limited improvement, mainly in the integration of data. A group 2 set of observables would require development of a next generation of satellites, reinforcement of routine ground and airborne measurement and the development and implementation of a data assimilation system.

The implementation of IGACO comprises two phases; short term group 1 observables (0-10 year, before 2013), and long-term (beyond 2013) for a comprehensive system comprising group 1 and group 2 observables. The long term phase requires immediate action of space and financing agencies now in order to fill the looming gap in satellite based observations after the present generation of research type satellites has run out of operational lifetime.

The IGACO team has produced a theme report that has been approved at the IGOS Partners meeting in May 2004. The information will feed into the GEO and GMES initiatives. Several CAPACITY partners play a leading role in IGACO.

European

GMES

Global Monitoring for Environment and Security (GMES) is a joint EC-ESA initiative, started in Baveno 1998, aimed at bridging the gap between scientific data produced and useful information needed by governments and the general public. The overall aim of GMES has been stated in the Final Report for the initial period 2001-2003 (1): “To support Europe’s goal regarding sustainable development and global governance by providing timely and quality data, information and knowledge. - This entails the capacity to have independent and permanent access to reliable and timely information on the status and evolution of the Earth’s environment at all scales, from global to regional and local.“.

In particular, the GMES information will support Europe in meeting its environmental obligations. It will contribute to the formulation, implementation and verification of the Community environmental policies, national regulations and international conventions. There is also a contribution to the security of citizens; forecasts of air pollution and UV radiation events and predictions of climate change and its consequences could be classed in this category. There is an overarching objective for GMES to contribute to sustainable development, both within the EU and globally. This requires an interdisciplinary approach.

The GMES action plan 2004-2008 (2) sets out to establish a GMES capacity by 2008, including a governance structure and funding strategy. Priorities selected for the core GMES capacity include support to the EC 6th Environmental Action Programme (3). Special reference is made to the GMES requirements for Environmental Policy monitoring for Climate Change and Air Quality policy. A number of CAPACITY partners are participating in the GMES working groups on national and European level.

European Commission FP5 and FP6 RTD programmes
The Framework 5 Research and Technology Development programme of the European Commission has commissioned the GMES-GATO (Global Atmospheric Observations) project to define a strategy for GMES to help develop an integrated global atmospheric observing system by 2008 [RD2]. The strategy assesses what the current European observation and modelling capabilities are, observations both from ground and from space, and describes how a more rationalised European monitoring system could be developed. Apart from the observing capability, it examines various aspects such as quality control, data storage and access, and the provision of useful information to parties concerned (end-users). The following issues are considered in relation to all aspects of atmospheric monitoring:

- Verification of compliance and success of implementation of Protocols
- Provision of near-real time information to public and scientific community
- Synergy of observation and modelling
- Quality, archiving and access
- Continuation of satellite observations beyond ENVISAT
- Development of a non-satellite monitoring system for GMES post 2008
- Provision of funding and national funding frameworks

European Commission Environmental Action Plan
The 6th Environmental Action Programme 2001-2010 (3) forms a framework for the European Community environmental policies and addresses a number of relevant issues, including Climate Change , Air quality, Sound knowledge and Involvement of (policy) data users. The principal European Community Plans, Directives, Council and Parliament Decisions on Climate Change and Air Pollution relevant to CAPACITY are within the province of the 6th EAP framework.

The EC White paper on Space, recently approved by the Commission and by the European Parliament (4), defines a future strategy for space activities within the EU, and is based on the benefits that space activities can bring to society and the citizens of Europe. The Earth Observation GMES programme was identified as one of the main areas of near and medium term investment. Priority will be given in developing GMES services in support of a number of areas, including "Atmospheric monitoring to contribute to understanding climate change, analysis of weather events and measurements of pollutants that damage human health. Services will provide real time information on atmospheric chemistry, pollution, aerosol and ozone components."

EUMETSAT
The EUMETSAT mission was recently broadened to deliver operational satellite data and products on climate monitoring as well as on meteorology. EUMETSAT is a strong supporter of GMES and foresees the need for investment in operational satellite systems to complement the current MSG and MetOp series of satellites and to provide continuity in the data after ENVISAT. With the GOME-2 and IASI instruments on the MetOp series of satellites (2005-2020) EUMETSAT will ensure continuity (as well as redundancy) on some of the data supplied by ENVISAT and by the EOS-Aura satellite.

EUMETSAT is also actively engaged in the definition of observational requirements for the next generation of satellites that must become operational in the 2015-2025 era. Here, short range forecasting of global air pollution is considered to be an important requirement for health and safety.

This would require high temporal resolution of observation in the range of 1 to 6 hrs. Proposals based on tropospheric trace gas measurements from Geo-stationary orbit are under study.

European Environmental Agency EEA
The European Environmental Agency (EEA) conducts environmental assessments and provides policy relevant information on climate change and air quality to the European Commission DG Environment, the European Parliament and Member States (31 members). Coordination between the EEA activities and CLRTAP/EMEP has recently been established through the EC Clean Air for Europe (CAFÉ) programme. The EEA works through Topic Centres, in this case the European Topic Centre of Air Quality and Climate Change (ETC-ACC), which consists of a consortium of national environmental institutes. The EEA requirements are driven by the EC 6th Environmental Action Plan [3], and the compilation of the 2005 report on the State and Outlook of Europe's Environment (SOER 2005). For observational data the EEA relies on the ground based measurement network. For Climate Change and Air Quality satellite data are expected to provide the global and European dimension not well covered by the ground-based network.

National programmes

A number national initiatives and programmes have served as a basis for the CAPACITY definition study.

References :

1. ESA PB-EO(2001)56 rev1, EC COM(2001)609 and EC COM(2001)264
2. COM (2004) 65 final
3. EC COM(2001)31final of 24.01.2001
4. EC COM (2003) 673.

Approach to an Integrated Observing System

In order to be able to meet the User Requirements on Air Quality and Climate Change, high accuracy information is required in the planetary boundary layer. This information cannot be retrieved from satellite measurements alone and must rely on a combination of ground-based *in-situ* and space based measurements. The combination of these measurements is achieved in a consistent way by assimilation of the various kinds of measurements into models and validating the analysis by independent measurements.

The Integrated Global Observation Strategy for Atmospheric Composition monitoring followed in this study and advocated by IGACO [RD1] comprises four components:

- Ground based data
- Airborne data
- Satellite data
- Assimilation of these data into Atmospheric Chemistry Transport models

It is expected that this approach will be able to provide high quality information in the planetary boundary layer and also in the free troposphere and in the stratosphere, that would not be feasible if relying on space or ground based observations in isolation.

Ground-Based data

WMO-GAW
The WMO Global Atmosphere Watch is an observational network for long-term measurements of atmospheric composition, including ozone, greenhouse gases and pollutant gases and particles. It is a key network for monitoring global atmospheric change. It forms part of the Global Climate Observing

System (GCOS). Many existing networks fall under the GAW umbrella and encompass global monitoring networks on greenhouse gases, ozone, UV radiation, aerosol, reactive gases, precipitation chemistry and radionuclides. For the stations within the GAW network a calibration scheme exists, guarantying a minimum quality of data from these stations.

NDSC
The Network for Detection of Stratospheric Change plays an important role in providing a link between ground based and space based observations because of the ground based remote sensing instruments it includes in the network. Validation of space based observations is more straight forward through ground based measurements of total column amounts as opposed to local concentration measurements.

NOAA-CMDL and *AGAGE*
Local concentrations of greenhouse gases are monitored by the NOAA-*CMDL* (Climate Monitoring and Diagnostics Laboratory) and *AGAGE* (Advanced Global Atmospheric Gas Experiment) ground networks.

EMEP
The Cooperative programme for Monitoring and Evaluation of the Long-Range transmission of Air Pollutants in Europe forms one of the main pillars on which CLRTAP rests (1). For EMEP stations a standardised quality scheme is operational.

1.EMEP/CCC Report 9/2003

Aerosol column and vertically resolved properties are derived from sun photometer data. The *PHOTONS/AERONET* network is based on standardised measurements using one type of sun photometer. Long-term ground based in-situ measurements derive mainly from EMEP. *EARLINET* is an EC FP5 supported European LIDAR network providing aerosol vertical profile measurements.

Airborne

Ozone balloon sondes are launched regularly from many stations around the world for many years, as part of the responsibility of meteorological organisations. These data provide high vertical resolution data on ozone and water vapour but are limited in temporal resolution and geographical spread.
Starting in 1994, in-situ measurements on commercial airliners have been performed on a regular basis. The first initiative was MOZAIC with measurements of ozone and relative humidity. Later, similar projects CARIBIC and NOXAR provide necessary data on additional species and extending geographical and temporal coverage . Currently these projects provide detailed in-situ observations of more than 60 tracer species, covering a large part of the globe. Europe is playing the leading role in this observational network.
For understanding ozone depletion in the Arctic, major field campaigns have been conducted under the EC 3rd, 4th and 5th Framework Programmes, e.g. the European Arctic campaigns EASOE, SESAME, THESEO, and VINTERSOL. These campaigns are continued under the EC 6th Framework Programme on a routine monitoring basis coordinated by the Ozone Coordinating Unit based in Cambridge UK.

Space-based

This decade many new Earth Observation satellites for Atmospheric Composition have and will come into operation, notably ENVISAT, MSG, MetOp, EOS Terra, EOS Aura and OCO. Exploitation of their data is now opportune; clearly *this is the decade of the data*. However, the use and usability of satellite data for environmental application is still in its early days. The Kyoto and CLRTAP protocols require data on processes that are taking place in the planetary boundary layer. One of the recent advances in satellite instrumentation has been the ability to probe the troposphere from space. For example, the nadir viewing instruments GOME and ATSR on the ESA ERS-2 satellite have demonstrated the feasibility of retrieval of data on tropospheric ozone, NO2, BrO, HCHO, SO2 and

aerosol. However, the accuracy and spatial resolution, in particular the resolution of the planetary boundary layer, is still far from what is required for Protocol verification.
The ESA ERS (1995-2003) and ENVISAT (2002-2007) satellites and associated data systems form the core of the current European observation capability. The EUMETSAT MetOp satellites series (2005-2020) provide long-term continuity for some of the data requirements. The ESA Data Processing and Archiving Centres (PAC) and the EUMETSAT Satellite Application Facilities (SAF) form the basic source of level 2 data. It should be recognised that these data products stop at level 2 (calibrated/validated trace gas and aerosol concentration distributions) and that the quality of these data is not always good enough for application in air quality and climate change areas.
The NASA EOS-Terra satellite (1999-present) and EOS Aura (2004-2010) will also form an important source of data. The future NASA research mission OCO (2007-2010) will play a key role in providing carbon dioxide data. CAPACITY partners have PI or co-investigator status in these US missions and therefore access and insight in the data.
Aerosol measurements from space are more complicated than gas measurements in that not only concentration but also size, shape and chemical composition need to be measured for their role in climate and air pollution applications. Measurements of aerosol optical density (AOD) from MODIS and ATSR presently form the basic source of aerosol data. The space based measurement capability for aerosol was severely reduced by the recent loss of the Japanese ADEOS-2 satellite carrying the French POLDER instrument. A future deployment of POLDER is foreseen on the Parasol platform (2005) as part of the NASA A-train. CAPACITY partners are involved in these activities.

CAPACITY partners have been actively engaged in the definition of elements of a future atmospheric composition observation system. Specific proposals have been submitted on a high temporal resolution air pollution mission in Geo-stationary orbit [RD11, RD12] and a high vertical resolution upper troposphere, lower stratosphere mission in Low Earth orbit [RD10].

Data Assimilation into Models

Modelling and data assimilation, bring together the large variety of measurements obtained from different sources to provide optimal temporal and spatial reconstructions of key atmospheric constituents. Such a synthesis yields invaluable information on the consistency and the quality of measurements so that trends, variability and sources and sinks of these species can be quantified. In turn, based on these results, improved models can be developed that provide better predictions as well as a better reconstruction of past changes.

CTM Models. A basic tool is an atmosphere chemical transport model (CTM). Such model is based on the physics of fluid dynamics and transport, input from an emissions module to provide data on man made and natural biosphere emissions, a chemical module, which may include hundreds of species and chemical reactions. More complex processes involving aerosols, liquid processes in cloud droplets, and reactions on the surface of solid particles, are treated through parameterisation. Such models of the atmospheric dynamics and chemistry have the ability to calculate missing and under-sampled parameters and to generate continuous and self-consistent fields of atmospheric trace constituents. The specific CTM's considered by CAPACITY will consist of the model TM3 by KNMI, the 3D NCAR-ROSE model by DLR, the CHIMERE model of CNRS, the IMAGE model at IASB/CNRS and the MOCAGE model by Météo-France.

CCM Models. Long-term descriptions of the atmosphere can be obtained with chemistry-climate models (CCM), where the evolution of atmospheric composition and climate is modelled simultaneously and interactively, taking account the feedbacks between chemistry and climate. Present models are reasonably successful, although there are weaknesses in the parameterisations, the emission scenarios assumed, and the chemical mechanisms employed. There is an inherent problem of averaging - using values within a model grid box, which markedly vary within the dimension of the box - this problem is equivalent to the problem of the representativeness of a particular measuring station for a model grid square, and indeed the representativeness of a satellite column measurement for the average concentration.

Data Assimilation. The integrated observation system will combine the information contained in the measurements and in the theoretical model by means of a data assimilation scheme in order to generate data of improved quality. Data assimilation heritage derives from the NWP development of weather forecasting models. It is based on the minimisation of the difference between model evolution and measurements (Bayes theorem). An essential element in the scheme is the quantification of errors that may originate from either measurement or model, and the gain in information content is continually assessed. The output will be the best available knowledge of the state of the atmosphere, which must however be validated by independent measurements.

Assimilation of satellite measurements of chemical species, notably stratospheric ozone, into an operational weather forecast system is a relatively recent development. It has been used in numerical weather prediction by ECMWF to significantly improve the assimilation of satellite radiances. It has been successfully applied by KNMI to forecast the evolution of the ozone hole and to forecast the UV exposure of the earth surface. Daily UV forecasts are delivered by a number of meteorological organisations, including CAPACITY partners Météo-France and KNMI, and form a highly visible demonstration of this technique.

New challenges in data assimilation and CTM model development are posed by the inverse modelling of emissions. An important application is the improvement of the greenhouse gas emission inventories derived from atmospheric concentration distributions as is currently pioneered by the EC FP5 RTD project EVERGREEN [RD16]. In the past, the application of this technique had been limited by the sparse data available from ground based stations and flask measurements. With the advent of space based measurements much better global coverage will be achieved. However, the improvement of the accuracy of space based measurements and how such remote observations relate to observed boundary layer and surface observations remains a critical challenge.

Air Quality forecast. The generation of an air pollution forecast or a chemical weather forecast is a further application of the integrated observation system. Utilization of air quality forecast models requires near-real-time chemical data acquisition, typically within three to six hours. For rapidly varying species, sampling must be frequent enough to capture these variations. For example, species that exhibit significant diurnal variation, like ozone, NO2, SO2, CO, aerosol, require measurements at sub-daily, ideally hourly, intervals. Building an operational system for chemical weather forecasting imposes challenging requirements on the timely delivery of the input data, the quality and consistency of the data, the quality and reliability of the output data generated, as well as the long-term continuity prospect of the entire system.

Ancillary data

The observation system defined needs to be self sufficient in that data needed to retrieve key observables need to be included in the set of requirements. For example, data on temperature and pressure distribution in the atmosphere are usually needed in order to retrieve atmospheric trace gas distributions. Furthermore, wind, humidity, clouds in various form and altitude (noctiluscent, mother of pearl, cirrus, cumulus etc), solar irradiance, albedo, vegetation and fire maps are ancillary data needed in a comprehensive observation system. The global coverage, temporal resolution and accuracy required often implies that dedicated satellite instruments are needed.
Meteorological data identified above are currently available from the Numerical Weather Prediction (NWP) model at ECMWF. This model is based on assimilated global observations of dedicated satellite and ground based instruments. The accuracy of the data is the best that can be achieved with available model and observation capability. For example, the ECMWF model is extended to cover the stratosphere upwards at increasingly fine vertical resolution. This has resulted in temperature accuracy better than 1 K throughout the troposphere and much of the stratosphere, except for special conditions such as the ozone hole where temperatures are accurate within a few degrees only. More accurate data would require a dedicated observation capability and thus cannot any longer be regarded as an

ancillary to the mission. In this study such data requirements are considered part of the mission and are specified in WP 2100.

On the other hand, atmospheric composition data are of relevance to other environmental science and application areas. For example, satellite data of the Earth surface must account for atmospheric effects in order to accurately retrieve surface properties. Observations of land change, ocean colour (for biological activity), coastal zone erosion, sea and land ice, vegetation fires, oil spills, algal blooms, chemical and nuclear accidents and conflict will be benefiting from better atmospheric composition data. In general, a Global Earth Observation System addressing environmental hazards, land mapping and ocean monitoring will benefit from ancillary Atmospheric Composition data [RD2, Ch6].

Outline of this document

The document is structured as follows. Indicated between brackets are the numbers of the work packages that are occasionally referred to in the different Chapters.

- Chapter 1: User requirements (WP 1000)
- Chapter 2: Geophysical Data Requirements (WP 2100)
- Chapter 3: Assessment of existing and planned space systems and ground networks (WP 2200)
- Chapter 4: New system elements (WP 2300)
- Chapter 5: Mission concepts for GEO (WP 3100)
- Chapter 6: Mission concepts for LEO (WP 3200)
- Chapter 7: Evaluation of Critical Space Segment Elements (WP 3300)
- Chapter 8: Evaluation of Critical Ground Segment Elements (WP 3400)
- Chapter 9: Overall Conclusions and Recommendations

Acronym List

AIRS	Atmospheric Infrared Sounder
AOD	Aerosol Optical Depth
AQ	Air Quality
ATSR	Along Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
CAFÉ	Clean Air for Europe
CALIPSO	Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations
CARIBIC	Civil Aircraft for Regular Investigation of the atmosphere Based on an Instrument Container
CLRTAP	Convention on Long-range Transboundary Air Pollution
CFCs	Chloro-Fluoro-Carbons
CREATE	Construction, Use and Delivery of a European Aerosol Database
CTM	Chemical Transport Model
DAEDALUS	Delivery of Aerosol Products for Assimilation and Environmental Use
DUE	Data User Element
DUP	Data User Program
ECMWF	European Centre for Medium-Range Weather Forecasts
EDGAR	Emission Database for Global Atmospheric Research
EEA	European Environmental Agency
EMEP	European Monitoring and Evaluation Programme
ENVISAT	Environmental Satellite
EPS	EUMETSAT Polar System
EUMETNET	European Network of Meteorological Services
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
EVERGREEN	Envisat for Environmental Regulation of Greenhouse Gases
ESA	European Space Agency
FCCC	Framework Convention on Climate Change
FOV	Field-of-View
FTIR	Fourier Transform Infrared
GAW	Global Atmosphere Watch
GCOM	Global Change Observing Mission
GCOS	Global Climate Observing System
GEO	Geostationary Orbit
GEOSS	Global Earth Observation System of Systems
GHGs	Greenhouse Gases
GMES	Global Monitoring for Environment and Security
GMES-GATO	GMES Global ATmospheric Observations (EU-GMES project)
GOME	Global Ozone Monitoring Experiment
GSE	GMES Service Element
HIRDLS	High Resolution Dynamics Limb Sounder
IASI	Infrared Atmospheric Sounding Instrument
IGACO	International Global Atmospheric Chemistry Observations
IGBP	International Geosphere-Biosphere Program
IGOS	Integrated Global Observing Strategy
IPCC	Intergovernmental Panel on Climate Change
LEO	Low Earth Orbit
MASTER	Millimetre-wave Acquisitions for Stratosphere-Troposphere Exchange Research
METOP	Meteorological Operational Polar satellites EUMETSAT
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MIR	Mid Infrared
MLS	Microwave Limb Sounder
MODIS	Moderate Resolution Imaging Spectrometer

MOPITT	Measurements of Pollutants in the Troposphere
MOZAIC	Measurements of Ozone, water vapour, carbon monoxide and nitrogen oxides by Airbus In-Service Aircraft
MSG	Meteosal Second Generation
MTG	Meteosat Third Generation
NMHC	Non-Methane HydroCarbon
NPOESS	National Polar-orbiting Operational Environmental Satellite System
NRT	Near-Real Time
NWP	Numerical Weather Prediction
ODS	Ozone Depleting Substances
OMI	Ozone Monitoring Instrument
OMPS	Ozone Monitoring and Profiling Suite
PAHs	Poly Aromatic Hydrocarbons
PAN	Peroxy Acetyl Nitrate
PBL	Planetary Boundary Layer
PM	Particulate Matter
POPs	Persistent Organic Pollutants
PROMOTE	Protocol Monitoring for the GMES Service Element
PSC	Polar Stratopsheric Cloud
SAGE	Stratospheric Aerosol and Gas Experiment
SCIAMACHY	SCanning Imaging Absorption SpectroMeter for Atmospheric CarograpHY
SSP	Sub-Satellite Point
TEMIS	Tropospheric Emission Monitoring Internet Service
TROPOSAT	Use and usability of Satellite Data for Tropospheric Research
UARS	Upper Atmosphere Research Satellite
UNEP	United Nations Environmental Program
UNFCCC	UN Framework Convention on Climate Change
UTLS	Upper Troposphere and Lower Stratosphere
VOCs	Volatile Organic Compounds
WCRP	World Climate Research Program
WHO	World Health Organisation
WMO	World Meteorological Organisation

1 User Requirements

1.1 Executive Summary

This work package identifies the user requirements for an Atmospheric Composition operational monitoring mission. The user requirements are formulated as high level data requirements responding to the need for information in the fields of stratospheric ozone and surface UV, air quality and climate change. The user requirements are derived from services delivered to users. It draws on the experience currently building up with users in the ESA GMES project PROMOTE. Here, a number of services in the areas of stratospheric ozone, surface UV and air quality are already being made operational. The services are delivered from specialised service centres that collect, process, integrate and archive the data. The services can be delivered near-real time or off-line. Underlying data are retrieved from satellite, ground based and airborne observations in combination with theoretical models. Use is made of the data assimilation technique, a statistical method that brings together measured and modelled data into a self consistent form. A global monitoring and forecasting system with spatial and temporal continuity is thus formed. This strategy is based on the integrated global observing strategy advocated by the IGACO group (ESA SP-1282). The requirements for Ozone/UV, Air Quality and Climate services are grouped into specific application areas: Protocol monitoring, forecasting and (scientific) assessment. This leads to a 3x3 matrix of services each with specific requirements.

1.1.1 Stratospheric Ozone and Surface UV

Stratospheric Ozone and Surface UV Protocol monitoring requirements stem from the Montreal Protocol and its subsequent amendments that regulate the release of ozone depleting substances into the atmosphere. The evolution of the ozone layer needs to be monitored over a period of decades. Also, the UV radiation incident at the earth surface needs to be monitored together with information on ozone, aerosol, cloud and surface albedo. Episodes of high UV exposure, dangerous to man, requires a forecast system that relies on Near Real Time (NRT) delivery of total ozone data. Numerical Weather Prediction has been improved by assimilation of NRT total ozone data.

Daily total ozone is required at 3% accuracy, 50 km horizontal resolution. Future requirements on now-casting and very short range forecasting in 2015-2025 have been formulated by EUMETSAT. A temporal resolution of 6 hrs with delay time of less than 3 hrs would be desirable to improve NWP.

For scientific assessment a broad range of measurements is required, including ozone depleting substances, polar stratospheric clouds and the key species in the catalytic ozone destruction cycles. The ozone profile needs to be known with vertical resolution of 2 km in the upper troposphere and lower stratosphere. The requirements for ozone assessment include the measurement and modelling of climate-chemistry interaction that influence the rate at which the ozone layer will recover.

The protocol monitoring and forecast requirements are similar to those met by current and planned operational satellite missions. For assessment these missions run short of the required species range and the required altitude resolution which requires new and advanced observational capability.

1.1.2 Air Quality

One of the important advances in satellite remote sensing of the past decade has been the ability to probe the troposphere. GOME and recently SCIAMACHY and OMI have revealed uncanny maps of global air pollution at increasingly detailed resolution. This capability has been quickly ceased upon by Environmental Agencies wishing to extend their observational capability. The information required at the planetary boundary layer is not readily accessible from satellite and requires an intermediate step involving data assimilation into models.

User requirements for AQ protocol monitoring are derived from the EC air pollution directives and the UN ECE Convention on Long Range Trans-boundary Air Pollution (CLRTAP). These include the measurement at ground level of aerosol and gases at city scale resolution. For aerosol the demand is for data on particulate matter (PM) at increasingly fine scale, ranging from 10 micron to 2.5 micron and possibly sub-micron size in future. For gases the interest is in ozone O3, nitrogen dioxide NO2, carbon monoxide CO, and sulphur dioxide SO2. Because of diurnal variation in these species, high temporal sampling of 1 to 2 hours is needed during day time when photo chemistry is altering the concentration distribution.

The interest in air quality forecast for health and regulatory reasons requires near real time delivery of data. Requirements on future now-casting and very short range forecasting in 2015-2025 formulated by EUMETSAT require day time measurements, night time measurements are desirable. Horizontal resolution for measurements of O_3, CO, SO_2, NO, NO_2, HCHO, PAN, VOC is: threshold 10 km and optimum 2 km. Vertical resolution requirements are: threshold tropospheric column and optimum 2 km. Temporal resolution is: threshold 2 hrs, optimum 30 minutes. Accuracy threshold 50%, optimum 20%, except for O_3 and CO which should have threshold 10% and optimum 5% accuracy.

For aerosol requirements are formulated for optical depth, size distribution, and single scattering albedo. Horizontal resolution ranges from threshold 5 km to target 0.5 km. Vertical resolution ranges from threshold total column to target tropospheric column and boundary layer (2 pieces of information). Temporal resolution is: 1 hrs threshold and 15 min target. Accuracy threshold 5%, target 1%, except for size threshold 30%, target 10%.

For air quality assessment and its long term evolution, the oxidising capacity of the atmosphere is the main driver of the observational requirements. Here, the hydroxyl radical OH plays a pivoting role that needs to be constrained by measurement of key species in the troposphere.

The outstanding requirements for Air Quality are thus; high temporal resolution, high horizontal resolution and sensitivity to the planetary boundary layer. These requirements are not currently met by existing or planned observation systems and present a challenge for future satellite and instrument development.

1.1.3 Climate

Climate protocol monitoring requirements derive from the Kyoto Protocol. It concerns the emissions of greenhouse gases (GHG) carbon dioxide CO_2, methane CH_4, nitrous oxide N_2O, and some minority gases such as sulphur hexafluoride SF_6 and HCFC gases not covered by the Montreal Protocol. Anticipating on future needs, also tropospheric ozone and aerosol are included in these requirements as well as the precursor gases carbon monoxide CO and nitrogen dioxide NO_2. The observational requirements stem from the need to narrow down the uncertainty in emission inventories. This includes both anthropogenic and biogenic sources and sinks. For climate prediction and climate assessment the emphasis is on the radiative effect of changing GHG and aerosol concentrations. The atmospheric layer most sensitive to these changes is the upper troposphere and the lower stratosphere which needs to be monitored at high vertical resolution.

Understanding climate chemistry interaction is the driver in climate assessments. Atmospheric chemistry plays an important part in controlling a number of important greenhouse gases and aerosol. This includes chemically active gases ozone, methane and water vapour. Aerosol form a particular challenge because of their high variability in space and time and the need to know additional parameters such as single scattering albedo and phase function in order to characterise their reflecting and absorbing properties. For the retrieval of GHG and aerosol emissions requirements are taxing in sensitivity at the planetary boundary layer. Here, CO_2 measurements are included in the baseline requirements. However, full requirements for emission retrievals are not included. Requirements for N_2O measurements are not included in the space segment.

These are long lived species that can be captured by ground based measurement. The requirements for climate assessment are characterised by high vertical resolution in the upper troposphere and the entire stratosphere for the species referred to and some tracer gases. This is needed in order to reveal the dynamics (Brewer-Dobson circulation) and vertical transport across the tropopause.

Although climate data relate to long-term (decadal) data records, there are technical advantages in having these data delivered near real time in order to allow on line assimilation in numerical weather prediction models. Numerical weather prediction models form the basis of many climate prediction models.

1.2 Introduction

1.2.1 Purpose

This document WP 1000 sets out the User Requirements for an Operational Atmospheric Chemistry Monitoring Satellite Mission. The word operational is used in the sense that a robust and reliably working service of good quality information can be established. The word monitoring is used in the sense that long-term continuity and consistency of the information is achieved. Long-term continuity in the data is essential in order to capture the changes and trends in atmospheric composition that occur on a time scale of several decades.

User requirements are defined at high level, identifying areas of application and needs for information to end users, including quality attributes. From these requirements for high level information, requirements for higher level data products (level 4 integrated data) are derived, specifying the spatial and temporal resolution, accuracy, timeliness and long-term continuity. This specification then forms the basis of WP 2100 in which requirements for sensor data products (level 2 data) are derived.

1.2.2 Background

Recently, a number of initiatives have come together which have benefited the CAPACITY study. These are

- IGACO (Integrated Global Atmospheric Chemistry Observations) forming part of the international partnership IGOS (Integrated Global Observation Strategy) is concerned with global environmental change issues. IGACO has recently issued a Theme report "The Changing Atmosphere" [RD1, 27 May 2004], which defines a strategy for a step-wise implementation of a future global observation system for atmospheric composition based on the integration of space, ground and airborne data into models.
- GEOSS (Global Earth Observation System of Systems), is an international initiative resulting from the first Earth Observation Summit (Washington 2003) following recommendations of the G8 Summit in Evian. At the second EO summit (Tokyo 25 April 2004), a framework document was adopted and at the third EO summit in Brussels, 16 February 2005 a 10-year implementation plan for GEOSS was approved.
- GMES (Global Monitoring for Environment and Security), is a joint EC and ESA programme which has recently concluded its initial period 2001-2003. It has defined an action plan 2004-2008 for establishing a GMES capacity by 2008. GMES is seen as a European contribution to GEOSS.
- The ESA GMES Service Element which includes a service for Atmospheric Composition named PROMOTE. This service can be seen as the practical implementation of user requirements, in that it provides experience with providing services on atmospheric composition to users and getting their feedback on the usefulness of these services delivered. The project ends in December 2005.
- The EC 6FP Space Integrated Project GEMS runs from 2005 to 2008 and will carry out research and development in atmospheric composition modelling and forecasting. It will provide the research and development basis for PROMOTE services.

The CAPACITY study responds to these initiatives by specifying in further detail the space segment of the atmospheric composition observation system and strives to provide input to the implementation plans for IGACO, GMES and GEOSS. It defines requirements aimed at meeting initial and future specifications of a GMES Service for Atmosphere. The time horizon for full operation of the space segment of the GMES service for atmospheric composition monitoring is the next decade 2010-2020.

1.2.3 Scope

This document is based on a vision, expressed by IGACO, that user requirements for atmospheric composition monitoring can only be fulfilled by adopting an integrated approach to the global observation system by combining data from ground-based, airborne and satellite systems into theoretical models. Only this approach will lead to the services satisfying end user's information requirements at ground level where emissions take place and where health and safety aspects are at issue. The approach will also provide for a self-consistent and comprehensive description of the atmosphere system.

The specification of User Requirements is a wide ranging process that builds on the heritage from similar studies performed in the past. In this report the requirements from existing studies will be traced and critically reviewed. As is already mentioned, this document draws on work carried out by the IGACO team in 2003 which findings are laid down in the Theme report "The Changing Atmosphere", recently approved by the IGOS-Partnership [RD1]. The IGACO report in turn draws on requirements specifications developed earlier for the World Meteorological Organisation Global Atmospheric Watch WMO-GAW programme [RD7]. The European organisation for operational meteorological satellites EUMETSAT, recently produced a position paper on Observation requirements for Now Casting and Very Short Range Forecasting in 2015-2025 that is very relevant to this study [RD4]. Similarly, the EUMETSAT study for Geo-stationary Satellite Observations for Monitoring Atmospheric Composition and Chemistry Applications in 2015-2025 [RD9] provides requirements for a successor to Meteosat Second Generation (MTG). For climate requirements reference is made to the draft Implementation Plan for the Global Observing Systems for Climate (GCOS) in Support of UNFCCC [RD8]. More specifically, the ESA study for greenhouse gas emission retrieval from space based measurements [RD 3] provides detailed requirements for a satellite system for climate monitoring. Proposals for the ESA Earth Explorer missions ACECHEM [RD10], GeoTrope [RD11] and TROC [RD12], provide feedback on satellite and instrument level data requirements that are relevant to the high level information requirements on stratospheric ozone, air pollution and climate.

The CAPACITY study takes into account the findings and recommendations of the joint EC and ESA GMES programme as formulated in the GMES Final Report for the Initial Period (2001-2003). The high level requirements for atmospheric composition monitoring follow from the Air Quality, UV and Climate Change Service categories identified. Reference is made to the EC study "Building a European information capacity for environment and security" [RD17]. The more demanding requirements for Air Quality and Climate Change services are the likely drivers in the definition of the future GMES space component for atmospheric composition monitoring.

At the start of the CAPACITY project the European user community involved in the project were given the opportunity to express their views. A User Consultation meeting was organised on 20-21st January 2004 at ESTEC. This workshop was attended by approximately 100 participants representing various user organisations, research organisations, and space industry. The result of this User Consultation meeting forms the basis of the User Requirement specifications developed in this document. Presentations are available from the CAPACITY web site.

Services already delivered to Users in the ESA GMES Service Element for Atmosphere PROMOTE provides hands-on experience on user requirements. These services are based on current state of the art observation, retrieval, data assimilation and modelling techniques. The service is continuously assessed by participating end-users and form a practical starting point for the definition of a future atmospheric composition monitoring system. By identifying the requirements that cannot be met by current and planned observation systems, the requirements for the future Operational Atmospheric Composition Monitoring System follow from there.

The recent ESA proposal for a GMES Earth Observation Component employs a similar logic in defining the space component (Sentinels) of the global observation system by relating these sentinels to the GMES Services currently developed under the Earth Watch GMES Service Element. It is noted that the definition of Atmospheric Composition Sentinels 4 and 5 is not as advanced as for the Sentinels 1, 2 and 3. The current schedule takes end 2012 as the timeline for the Sentinels 1, 2 and 3 to enter into operation. For Sentinels 4 and 5 the situation is yet to be decided and may start phase C/D activities in 2012 only. The CAPACITY study is consistent with this ESA time schedule which calls for preparatory activities in defining the space segment in 2005 (ESA/PB-EO(2004)48 rev.1 of 14 May 2004, ESA/PB-EO(2005)54 of 11 May 2005).

1.2.4 References

Applicable Documents

[AD1] ESA ITT AO/1-4273/02/NL/GS of 7 November 2002, including Statement of Work EOP-FS/0647 of 25 July 2002

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[RD2] GMES-GATO A European Strategy for Global Atmospheric Monitoring. 6th Framework Programme report EUR 21154 (2004). ISBN 92-894-4734-6.

[RD3] The potential of space borne remote sensing to contribute to the quantification of anthropogenic emissions in the frame of the Kyoto Protocol, by Francois-Marie Breon, Ph Peylin et al, ESA study 15427/01/NL/MM, 13 May 2003.

[RD4] EUMETSAT position paper on Observation Requirements for Now Casting and Very Short Range Forecasting in 2015-2025. B W Golding, S Senesi, K. Browning, B Bizzarri, W Benesch, D Rosenfeld, V Levizzani, H Roesli, U Platt, T E Nordeng, J T Carmona, P Ambrosetti, P Pagano, M Kurz. VII.02 05/12/2003, 28 February 2003.

[RD5] Group on Earth Observation (GEO), Report of the Subgroup on User Requirements and Outreach, 22 March 2004

[RD6] Manual on Volcanic ash, radioactive material and toxic chemical clouds, International Civil Aviation Organisation, Chapter 6, Doc 9691-AN/954, first edition 2001.

[RD7] WMO/CEOS report on a Strategy for Integrating Satellite and Ground-based Observations of Ozone. WMO Global Atmosphere Watch report 140, WMO TD No 1046, 2000.

[RD8] GCOS Implementation Plan for the Global Observing Systems for Climate in Support of the UNFCCC, draft report May 2004.

[RD9] Geo-stationary Satellite Observations for Monitoring Atmospheric Composition and Chemistry Applications, by Jos Lelieveld, Mainz, January 2003. EUMETSAT study for Meteosat Third Generation 2015-2025.

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[RD11] GeoTROPE, Geo stationary Tropospheric Pollution Explorer, by John P Burrows et al. Proposal in response to ESA 2nd call for Earth Explorer Opportunity Missions. COM2-32, 8 January 2002.

[RD12] TROC, Tropospheric Chemistry and Climate mission by Claude Camy-Peyret et al. Proposal in response to ESA 2nd call for Earth Explorer Opportunity Missions. COM2-35, 8 January 2002.

[RD13] WMO rolling requirement web site http://alto-stratus.wmo.ch/sat/stations

[RD14] Report of the WCRP satellite working group on update of space mission requirements for WCRP", Informal Report No. 8/2003, June 2003

[RD15] Air pollution in Europe 1990-2000. EEA Copenhagen, 2004 ISBN 92-9167-635-7. Environment in the European Union at the turn of the century, EEA Copenhagen 1999. ISBN 92-828-6775-7 and Appendix "Facts ad findings per environmental issue", ISBN92-9167-131-2.

[RD16] EVERGREEN, EC FP5 project EVG1-CT-2002-00079 coordinated A P H Goede. Project duration 2003-2006. For information see www.knmi.nl/evergreen

[RD17] Building a European information capacity for environment and security. A contribution to the initial period of the GMES Action Plan 2002-2003, by B K Wyatt, D J Briggs and P Ryder. DG Research report EUR 21109, ISBN 92-894-5000-2 (2003)

[RD18] Climate Chemistry interactions. Report from the joint SPARC/IGAC workshop, Giens, France, 3-5 April 2003. IGACtivities Newsletter, No 30, June 2004. SPARC Newsletter No 21, July 2003.

1.2.5 Sections Overview

Section 1.3 of this document classifies in general terms the areas of application for atmospheric composition monitoring and the need for information required in each area. Three main areas of application are identified: Stratospheric Ozone and Surface UV, Air Quality, and Climate Change. The required information is grouped into monitoring requirements, forecasting/near real-time and understanding. Subsequently, the relevant Earth Observation programmes and initiatives are described, both on an international and on a European level. The section concludes with an approach to an Integrated Observation System.

In Section 1.4 the user requirements are grouped per application. For each application the policy driver is identified and the existing and planned observational systems and models are reviewed. Requirements for monitoring, forecasting and understanding are developed by critically reviewing existing requirements and new requirements arising out of initial GMES Services. The section concludes with a specification of the services required by end user in the next decade (2010-2020).

1.3 Areas of Application

1.3.1 The Problem

The composition of the Earth atmosphere is changing, as long-term observations have shown. Human influence is clearly discernable, in some cases firmly established. The change in atmospheric composition induces change in climate, UV exposure and air quality. This change in turn has important (often adverse) consequences for human health and safety, balance of the eco-system and socio-economic conditions. To understand, predict and control environmental change is one of the main challenges of the 21st century.
Three areas may be distinguished in atmospheric change: Stratospheric Ozone/Surface UV, Air Pollution, and Climate Change. The global nature of the problem requires a worldwide coordinated approach. Indeed, in all these areas international Conventions and Protocols are in place or in preparation. The aim of these Protocols is to stem or reverse adverse environmental change. To be effective, these Protocols require timely, reliable and long-term information for assessment, monitoring and verification purposes.
In addition to the need to ascertain the effectiveness of Protocols, there is a need to predict future change. Daily forecast systems are presently emerging in various stages of development. A number of local and national authorities are already providing air quality and UV forecasts to serve public awareness and provide advance warning systems similar to the weather forecast service. On a different level, an intense research effort is directed at climate predictions and understanding the consequences of global change. The quality of predictions very much depends on valid theoretical models and accurate measurements of the state and evolution of the atmosphere.
Observational data and theoretical models together result in increased understanding of atmospheric change. This synthesis is needed for policy assessment and, in general, to advance our knowledge. Table 1.1 summarizes the three areas of atmospheric change together with relevant applications. Broadly speaking, these areas are arranged in descending order of maturity and feasibility, considering their status of implementation and effectiveness of Protocols, and the available means for independent verification.

Environmental Theme/ Service	**Stratospheric Ozone/Surface UV**	**Air Quality Local Regioanl, Contin**	**Climate-Atmosphere Composition int**
Protocols	**UNEP Vienna** **Montreal and sub Prot** **CFC emission verific** Strat ozone halogen trend monitoring	**UN/ECE CLRTAP,** **EMEP/Gothenb Prot** **EC Directiv EAP/CAFE** **AP emission verification** **AP trend monitoring**	**UNFCCC Rio Conv** **Kyoto Protocol** **GHG/aeros emiss verific** **GHG/aerosol distributio** **trend monitoring**
Forecast	**Stratospheric O3** **Surface UV** **NWP**	**Local Air Quality (BL)** **Chemi Weather (BL/FT)** **Aviation routeing (UT)** **Health Warning (BL)**	**Climate scenarios** **NWP reanalysis**
Assessment	**WMO O3 assessments** **UV health/bio effects** **global observations** **chemistry transp mod** **stratosphere chemistry** **UV radiative transp**	**UNEP, EEA assessments** **Health and safety effects** **Global, regio, local, obsv** **Long range transport** **Regio/local BL models** **Tropsperic chemistry**	**UN IPCC assessments** **Socio-Econom effects** **Long-term global observ** **Chemistry-climate int** **Radiative Forcing Mod** **Source attribution**

Table 1.1. *Application Areas in Atmospheric Chemistry*

1.3.2 The Need for Information

The need for information on atmospheric composition is driven by the potentially huge impact that global atmospheric change has on human health and safety, eco-system balance and socio-economic development.
High level socio-economic benefits identified [RD5] include:

- Understanding environmental factors affecting human health and well-being
- Understanding, assessing, predicting, mitigating and adapting to climate variability and change
- Improving weather information, forecasting and warning
- Improving management of energy resources

Direct needs for atmospheric composition information derive from monitoring and verification requirements of Protocols designed to regulate and mitigate the effects of human induced atmospheric change. This information is often needed on a country (signatory) by country basis. There is a need for independent global information for Protocol verification, separate from reporting obligations by individual signatories. This need calls for the ability to probe the atmospheric boundary layer on a global scale at high spatial and temporal resolution.

The process of policy formulation that leads to the implementation of Protocols is a multi-stage process which starts with the scientific discovery of change, the assessment and understanding of the issues involved, checked by the usual process of scientific scrutiny and independent verification. Good quality observations and reliable theoretical models are essential at this explorative stage.
This stage is followed by the political process of policy formulation and appraisal of policy. Autonomy and self-reliance of the European Union and Member States requires the ability to carry out independent investigation and assessment of environmental and climate issues. This is a strategic need for reliable environmental and climate information to be available at the negotiating table when politicians and policy makers need to decide on new policies. Access to high quality environment and climate data at all levels is required in order to be effective in policy implementation and verification.

Forecasts are necessary in order to anticipate episodes of risk to health and safety and to provide advance warnings to the public and the responsible authorities. Predictions of long-term environmental change are necessary in order to abate and mitigate the socio-economic consequences and to formulate policy and research agendas for sustainable development. Here, information based on a combination of measurements and models turns out to be necessary, and in the case of forecast, the delivery that information needs to take place in near-real time.

The need for stratospheric ozone information derives from the harmful effects of excess UV-B dose on health and biosphere. The Montreal Protocol calls for quadrennial ozone assessments and monitoring of stratospheric ozone concentrations and emissions of ozone destructing substances. Forecast of stratospheric ozone and surface UV prediction are possible and necessary in order to issue warnings and raise public awareness. Understanding of the ozone layer behaviour includes chemistry–climate interaction which is a subject of scientific research. Continued assessment and improvement of regulatory action is needed until the recovery of the ozone layer is a fact, currently not expected to happen before 2050.

The need for air pollution monitoring and forecast is driven by health and safety directives and conventions. The Convention on Long-Range Trans-boundary Air Pollution (CLRTAP) and several EC directives regulate the emission of air pollutants. Air Quality forecasts are important to serve as health warning in polluted areas. Environmental agencies need the AQ information in order to support implementation of regulatory actions on emissions from sources such as vehicular traffic and electric power generation. Reliability, timeliness, continuity and quality of this information is important. The temporal and spatial scale of requirements poses a challenge to both observational and modelling capability, ranging from street level to continental transport and from diurnal variability to decades of chemical lifetimes.

The need for climate information and prediction stems from the impact of climate change on society which can be enormous. Policy on greenhouse gas regulation will deeply affect the energy resource management, the transport sector and the economy as a whole. The UN Framework Convention on Climate Change (UNFCCC) adopted at the Earth Summit of Rio de Janeiro in 1992 and the resulting Kyoto Protocol (1997) commits the signatories to cut emissions of greenhouse gases by 8% in the period 2008-2012 compared with 1990 levels. The EU and some hundred other nations have ratified the Protocol, but major players like the USA have not, whereas developing nations like China and India are not committed. Climate predictions are limited by a range of uncertainties depending on economic development scenarios assumed and on the validity of models employed to describe the Earth System. Understanding climate change includes the chemistry climate interaction at all levels in the atmosphere, indeed in the entire System Earth. This subject is one of the great challenges for future global observation and modelling development.

1.4 User Requirements per Application

1.4.1 Stratospheric Ozone and Surface UV

Policy Stratospheric Ozone

The discovery of the ozone hole and the scientific understanding of the processes that lead to the depletion of ozone have resulted in the Vienna Convention for the Protection of the Ozone Layer (1985) and the Montreal Protocol on Substances that Deplete the Ozone Layer (1987). Subsequent amendments and adjustments of this protocol are based, and will be based on current scientific, environmental, technical, and economic information. To provide that input to the decision-making process assessments were carried out; the UNEP-WMO Scientific Assessment of Ozone Depletion in 1989, 1991, 1994, 1998 and 2002.

Ozone Observations

The ozone assessments are based on the long-term monitoring of the ozone layer and on observations of the abundance of ozone depleting compounds. Measurements are made from the ground, from aircraft, from balloon and from satellites. Ground-based stations form part of the WMO-GAW and NDSC network (e.g. Dobson, Brewer, DOAS, ozone sondes, lidar, microwave). Major field campaigns have been conducted over the Arctic from 1991 onward (e.g. the European EASOE, SESAME, THESEO, and VINTERSOL campaigns) deploying balloons and aircraft in-situ and remote sensing instruments. Commercial aircraft have carried out on a regular basis in-situ measurements of over 60 trace species covering a large part of the globe from 1994 onward (MOZAIC, CARIBIC, NOXAR). To date, satellites play an increasingly important role in the ozone assessment.

The series of TOMS instruments have been crucial in monitoring the changes in ozone on a global scale from 1979 onward. The accuracy of the TOMS total ozone data has been continuously improved. The new version 8 shows considerable improvement compared with its predecessor especially in the Southern hemisphere. Other US satellite instruments measuring ozone are SBUV/2 (since 1979), SAGE (1983) and TOVS (1985).

The European contribution to ozone monitoring with satellites started in 1995 with the GOME (Global Ozone Monitoring Experiment) on the ESA ERS-2 satellite. The higher spectral resolution of GOME compared with TOMS allows the use of DOAS –Differential Optical Absorption Spectroscopy - to retrieve trace gas total column density. The official GOME total ozone algorithm (GDP) has been improved several times since its first version 2.0, which appeared in 1996. The latest version GDP 3.0, issued in 2002, improves the match with TOMS vs8 to within a few percent, except for some Antarctic areas in polar spring. The cause of this discrepancy is expected to be resolved soon.

The ozone measurement series in the UV-visible spectral range will be continued with SCIAMACHY on Envisat (2002), OMI on EOS-AURA (2004) and GOME-2 on the METOP 1 (2005), 2 and 3 series. Recently, the NASA mission QuickTOMS failed. The currently operational Earth Probe TOMS instrument has been degrading. The GOME instrument has stopped producing global data from July 2003 onward due to satellite data recorder failure. As a result the ENVISAT SCIAMACHY instrument now plays an important role in filling the gap to OMI and GOME-2 both in ozone monitoring and forecast.

Ozone Observations Assimilated in Models

The usefulness of the total ozone data improves considerably if the data is provided at regular temporal and spatial intervals. Satellite measurements, however, are taken at overpass times and on orbital tracks with sampling constraints. Data assimilation is a technique that mixes information from models and measurements to produce output data of optimal spatial-temporal spread and known

accuracy. Total ozone assimilated into general circulation models (numerical weather prediction models) and chemistry-transport models was pioneered in the EU SODA project (1998) and is further advanced in the EU 5th FP project GOA (2002) and 6th FP project ASSET (2004-2007). The assimilated global ozone distributions form an important source of information for the ozone assessments carried out by WMO and UNEP.
Medium-range (up to 10 days) forecasts of ozone, based on the assimilation of near-real time ozone satellite measurements, have become available in recent years. Current ozone forecasting systems have been shown to produce meaningful ozone distributions for forecast periods of up to one week. Such ozone predictions are important for UV forecasting and for the prediction of large and rapid ozone variation such as excursions and break-up of the ozone hole, and the occurrence and evolution of "mini-ozone hole" events. For example, the spectacular break-up of the Antarctic ozone hole in the period 23-28 September 2002 was predicted successfully more than one week in advance by the ozone forecasting system of the KNMI.

1.4.1.1 Stratospheric Ozone Requirements

Requirements for operational observations of stratospheric ozone are in a rather mature state. They are formulated in the WMO Global Atmosphere Watch report [RD7], where also integration of ground and space based data is proposed. Prior to this report, ozone space measurement requirements have been iterated during the definition of GOME-2 and OMI for application on the EUMETSAT operational MetOp satellite (OMI User Requirements document, 1996). The ACECHEM study [RD 10] focuses on the ozone–climate interaction taking place in the lower stratosphere and upper troposphere part of the atmosphere. The recent IGACO report [RD1] focuses on the integration of observations from ground, air and space into models.
Threshold and Target requirements have been formulated for total ozone, the lower troposphere, the upper troposphere, the lower stratosphere and the upper stratosphere and mesosphere. Requirements formulated in these reports are in broad agreement.
For total ozone these requirements are typically (threshold to target from RD7):

- Horizontal resolution: 100 to 10 km
- Vertical resolution: 5 to 0.5km
- Temporal resolution 24 hrs to 6 hrs
- RMS error and bias each 5% to 1 %
- Trend detection 0.1% per year

More challenging requirements apply to the distinct vertical layers of the atmosphere (LT, UT, LS and US) where a 5 km threshold to 0.5 km target vertical resolution of the ozone distribution is required.

Montreal Protocol monitoring and treaty verification

The Protocol monitoring activities should lead to accurate information on the future evolution of the ozone layer. These activities include long-term monitoring of global concentration distributions of total ozone, monitoring of columns of ozone depleting substances; CFC’s and their replacement HCFC’s, halons, and a number of chlorine and bromine compounds representative of the various stages in the chemical reaction cycle [RD7]. For treaty verification, the sources of Ozone Depleting Substances (ODS) need to be identified and quantified. This can be done from bottom up country wise official figures like this is done today. However, some independent verification based on satellite measurements would be desirable. This can be achieved by inverse modelling of the CFC concentration distribution. Owing to their long chemical lifetime and hence their fairly uniform global distribution, inverse modelling results to date are not very accurate. Accuracy is however required because there are indications that certain countries do not abide by Protocol rules.

A challenging task but certainly needed for better policy information is the monitoring of height distribution of ozone and ODS compounds, in addition to total column information. This is necessary in order to separate the troposphere ozone component (pollution), from the stratospheric component relevant to the Montreal Protocol. For the ODS the altitude information indicates the effectiveness of treaty implementation and is therefore required. Certain active chlorine and bromine components (ClO and BrO) are needed as indicators of the severity and extent of ozone depletion. concentration distribution, size and chemical composition of polar stratospheric cloud (PSC) is needed for their active role in ozone depletion.

Stratospheric Ozone Forecasting

Observations of total ozone are currently assimilated in the Numerical Weather Prediction system of ECMWF with the aim to improve radiances and heating rates in NWP modelling and to provide input to surface UV forecasting. Requirements on future now-casting and very short range forecasting in 2015-2025 have recently been formulated by EUMETSAT [RD4]. These include observational requirements for total ozone column measurements for improved warnings of UV exposure under clear skies. These warnings can be considerably improved if total ozone observations were available at 5% accuracy, 10 km horizontal resolution and 1 hrs temporal resolution. Near real time availability of data (3 hrs) is required in addition to the above specification. See also Surface UV Requirements below.

One of the uncertainties in the production of a reliable ozone forecast is the coupling between the stratosphere and the troposphere, in particular the magnitude of the vertical transport of ozone across the tropopause. Here correlating species, such as CO, HCl, CH_4 and N_2O can serve as a proxy for ozone transport. Observation of these common tracers is a means to quantify stratosphere-troposphere exchange, in particular tropical tropopause layer.

Understanding of Stratospheric ozone

Better understanding of the ozone layer evolution and the role of the ozone depleting substances requires data for validation of models. Part of these data can be supplied by dedicated field campaigns focussing on process studies. This includes detailed measurements of the catalytic cycles implied in stratospheric ozone chemistry (the hydrogen, nitrogen and chlorine/bromine cycles) at specified time period in the year and region on the globe. Other data have to be obtained continuous and on global scale. Also data on (vertical) transport are needed and may be supplied by measurement of tracer gases such as N2O. Requirements formulated in the IGACO report [RD1], the ACECHEM study [RD10] and the WMO-GAW [RD7] are in broad agreement.

The IGACO report requires, besides ozone information, information on the following trace species: water vapour, active nitrogen (NO_x), reservoir (HNO_3) and source species (N_2O), active halogens (BrO, ClO, OClO), reservoir (HCl, $ClONO_2$) and sources (CH_3Br, CFC-12, HCFC-22), aerosol optical properties, and methane. In addition, a number of physical parameters are required (temperature, pressure, wind speed, cloud height, cloud coverage, albedo, lightning, solar radiance). Horizontal resolution is in the order of 50 to 250 km in the UTLS region of interest, vertical resolution ranges from 0.5 to a couple of km and accuracy ranges from a few to 10%.

The ACECHEM requirements are in broad agreement except for more emphasis being placed on the measurement of cirrus and polar stratospheric clouds.

1.4.1.2 Stratospheric Ozone Services

Requirements are aimed at services to be delivered to end-users. The following user organisations have been consulted:

- WMO
- ECMWF

Services below are based on current developments taking place in the GMES service for Atmosphere PROMOTE. Anticipated future requirements are developed in consultation with end-users.

Stratospheric Ozone Monitoring

Primary product for Protocol Monitoring (accuracy):

Accurate total ozone long time series 1979-2020. Total ozone time series retrieved from TOMS, GOME, SCIA, OMI, GOME-2, IASI, TES at 1% accuracy (no jumps between different sensors, also high latitude data).

Forecasting (Daily ozone field assimilated in CTM model)

Primary products for Forecast (accuracy):

(a) Daily total ozone (1%)
(b) Total ozone 5-10 day forecast at 3hrs interval (1%)
(c) Daily 3D ozone profiles (5%)
(d) Daily troposphere ozone column (10%)

Understanding the evolution of stratospheric ozone

Primary product for Understanding (accuracy)

(a) Daily total ozone (1%)
(b) Total reactive chlorine and bromine loading of the atmosphere (15%)
(c) Key components from catalytic cycles (HO_x, NO_x, ClO_x)
(d) Stratospheric H_2O, CH_4, and aerosol/clouds

1.4.2 Surface UV

Ultraviolet radiation, in particular UV-B (280-315 nm), has an important impact on the environment and on human health. Biochemical cycles (carbon and nitrogen), plant eco-systems, animal habitat, survival of pests and effectiveness of pesticides, are adversely affected by increased levels of UV radiation. Also aquatic organisms, such as phytoplankton, zooplankton, larval crabs, shrimps, juvenile fish are affected. Since these organisms are at the basis of the food chain, increased UV levels would adversely affect the entire aquatic eco-system. Over-exposure to UV radiation presents a global health concern and plays a major role in the annual 2 to 3 million non-melanoma skin cancers and 132,000 malignant melanomas. UV can cause or accelerate cataract development, may reduce the effectiveness of the immune system leading to decreased resistance in disease or reduced effectiveness of childhood vaccinations.

The level of surface UV radiation depends on a number of atmospheric constituents (gases especially ozone, aerosol and cloud) and on surface albedo (snow and ice cover, sun glint). In order to monitor and forecast UV-B, precise measurements of these parameters must be made. A distinction between urban and rural areas is important and hence good spatial and temporal resolution is required.

The depletion of the ozone layer leads on the average to an increase in the ground level UV-B radiation, because ozone features a strong absorption band in this spectral range (Hartley band). The past decades have shown, in many areas, an increase in surface UV-B radiation. The EEA reports in its environmental assessment of 1999 [RD 15] up to 10% increase in erythemal UV dose from 1980 to 1997 in certain Western European areas. Models predict that Arctic ozone loss is likely to peak around 2015-2020. This will have an impact on the levels of UV-B radiation over Europe in spring which are likely to increase.

Increased levels of UV may enhance the oxidising capacity of the troposphere, through increased photo-chemical activity producing the hydroxyl radical OH. Hydroxyl, being central to many chemical cycles, will affect the concentration of other species (O_3, H_2O, CO, CH_4, and other hydrocarbons) in the troposphere. On the other hand, recovery of the ozone layer may reduce photochemical activity in the troposphere and thereby reduce the cleansing of air pollution and greenhouse gas emissions. This chemistry interaction links the application areas of stratospheric ozone with those of air quality and climate.

Surface UV Policy

The United Nations Conference on Environment and Development (UNCED, 1992) under Agenda 21[1], produced a declaration on activities to be undertaken mitigating the effects of increased UV radiation. It recommends to undertake, as a matter of urgency,

- research on the effects of increased levels of ultraviolet radiation on human health as a consequence of stratospheric ozone depletion, and, on the basis of the outcome of this research,
- to take appropriate remedial action to mitigate the above mentioned effects on human health.

Current evidence suggests that people's sun-seeking behaviour constitutes the most important individual risk factor for UV radiation damage. WHO, in collaboration with the United Nations Environment Programme (UNEP), the World Meteorological Organization (WMO), and the International Commission on Non-Ionizing Radiation Protection (ICNIRP), developed and published the Global Solar UV Index in 1995. The UV Index (UVI) is an important measure to raise public awareness on the risks of excessive exposure to UV radiation and the need to adopt protective measures, see also COST-Action 713 (2001).

[1] Agenda 21 is a comprehensive plan of action to be taken globally, nationally and locally by organizations of the United Nations System, Governments, and Major Groups in every area in which human impacts on the environment.

The UV Index (UVI) is a dimensionless quantity proportional to the clear-sky UV irradiance, and is defined as the integral over the spectral UV irradiance incident on a horizontal plane in W/m^2 nm weighted by the CIE erythemal action spectrum[2] . The index is unity at 25 W/m^2 and zero at zero irradiance. The UVI refers to local solar noon when the UV irradiance is highest. Clouds are not taken into account. The higher the index, the greater the risk for damage to the skin and the eye, and the less time it takes for damage to occur.

In a number of countries, the media present the weather forecast together with expected UV radiation levels for the following day. Here, emphasis is placed on the time of day when the UV radiation level is highest. The intensity is normally computed for cloud free conditions. A more realistic measure of the UV exposure is the UV dose (kJ/m^2). This parameter is a measure for the total exposure during the day and involves integration from sunrise to sunset. The UV dose should also take into account the important effect of clouds. This necessitates a specific choice for the prediction of cloud cover during the day. Various algorithms have been developed that obtain the necessary input parameters from a variety of sources.

Surface UV Observations

Surface UV is governed mainly by extraterrestrial solar flux, solar elevation, cloud distribution and properties, snow cover, and the ozone column density. To a smaller degree, it is influenced by ozone profile shape, surface albedo, aerosols and ground elevation. Surface UV can only be measured directly by instruments on the ground, mainly sun photometers. Satellites do not measure surface UV directly, but provide input to radiative transfer computations, usually total ozone. Note that the satellite overpass time may not be optimal for the UV index calculation, e.g. too late or early to be representative for noon conditions. The extraterrestrial flux, solar elevation and altitude can be determined accurately. The remaining factors to be determined are the cloud parameters, ozone profile shape, surface albedo and aerosols.

Model computation of Surface UV

The UV index is computed using total ozone column density overhead, the distance from Earth to sun and a database of the Earth surface altitude and albedo. The computation uses a parameterisations or look-up tables based on empirical relations or radiative transfer computations. These off-line radiative transfer computations use climatologically values for surface albedo and aerosol loading. Recent developments include methods for determination of the surface albedo over snow and ice covered areas and take into account the effects of clouds

1.4.2.1 Surface UV Requirements

Surface UV requirements stem from the (human) health issues described above. Better UV-B measurements and warning systems will reduce the incidence of skin cancer and cataract. Requirements have been formulated in [RD4]. The UV services envisaged for the GMES Service Element for Atmosphere respond to needs of the UNCED requirements. These include both monitoring and forecast requirements. The most challenging task lies in the conciliation of the direct measurement of surface UV by sun photometers and the calculated surface UV from satellite measurement, the so-called closure experiments. For establishing the actual UV dose rate incident on human beings and biological organisms the effects of cloud and aerosol need to be incorporated in models.

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[2] The CIE spectral action function has been proposed by McKinlay & Diffey (1987) and adopted as an international standard by the International Commission on Illumination (CIE). It is modelled for the susceptibility of the Caucasian skin to sunburn.

Surface UV Monitoring

Surface UV index as well as UV dose need to be monitored for chemistry and biological models. The EUMETSAT position paper on observation requirements for now casting and very short range forecasting [RD4] states the following requirements (threshold/target):

- Total column ozone (100km/10km, 1d/1hr)
- Total column aerosol (50km/10km, 1d/1hr)
- Total cloud water (50 km/10km, 1hr/5min)
- Surface UV albedo (10km/1km, 1mnth/1day)
- NO_2 and other gaseous absorbers (10 km/10km, 1d/1hr)
- Ozone profiles (50km/10km, 2km/0.5km, 1d/1hr)

These requirements are deemed necessary for improvement of model predictions.
In the health sector requirements are governed by the needs of epidemiological studies on skin cancer and skin protection. On the latter there is a commercial interest from the beauty industry.

Surface UV Forecasting

In addition to the requirements for ozone forecasting and UV monitoring, near real time requirements apply to the provision of cloud, aerosol and gas absorption specified above (threshold/target within 3hrs/1hr, cloud within 30min/5min). WHO requirements are confined to UV index referring to clear sky conditions at local noon. It is considered that, while clouds are important, they are so variable that cloud observations would make little contribution to forecast accuracy. The EUMETSAT position paper [RD4] requires the total column of aerosol, being more persistent than clouds, with threshold accuracy better than 25%, 50 km horizontal resolution and 1 day temporal resolution threshold.
Development of mobile phones is expected to allow user specific UV exposure time and warning to be issued. Automatically updated now-casts of personalised sunburn time at the location of the enquirer will become possible in future.

Understanding of Surface UV

So-called closure experiments try to reconcile satellite measured solar irradiances at the top of the atmosphere with measured radiances at the Earth surface propagated through the atmosphere by atmospheric radiance transfer models. These measurements are relevant for the understanding of surface UV but also to the broader field of climate radiative forcing. Differences in surface irradiance in the order of tens of W/m^2 are generated by the presence of aerosol, both absorbing and scattering as well as their indirect effect on cloud formation.. These aspects need to be quantified and taken into account in the future radiative transfer models. Assimilation of surface based and space based data maybe needed in order to establish a consistent long-term data record of surface UV-B radiation.
Specific requirements for monitoring surface UV and establishing dose rates stem from users such as dermatologists for application in epidemiological studies. Here, region specific and time period specific information is required to establish, for example, real-time cumulative UV-B exposure of patients at their physical location.

1.4.2.2 Surface UV Services

Surface UV services are developed in consultation with the following user organisations involved in he ESA GMES Service for Atmosphere:

- SYKE (Finish Environmental Agency)
- RIVM (Dutch Agency for Public Health and Environment)
- BVDD (German professional society for dermatologists)

UV monitor long time series 1979-2020

Primary product for Protocol Monitoring:
UV index (clear sky) time series, global and regional maps, monthly/seasonal averages, 1 index point accuracy.

UV dose (clouded) time series, global and regional maps, monthly/seasonal averages, 25W/m2 CIE weighted accuracy.

UV forecast

Primary products for Forecast:
UV index (clear sky) daily forecast, 1 index point accuracy
UV surface irradiance from assimilated ozone fields daily forecast for 5-10 day in advance, 1 index point accuracy
UV surface irradiance taking into account the effects of aerosol and albedo
Personalised mobile telephone technology based sunburn time

UV understanding

Primary product for Understanding (accuracy):
Total dose taking into account clouds and aerosol (1 index point accuracy)
Closure experiments solar irradiance and surface radiance (1% accuracy)
Validation of space measurements through ground based network of sun photometer measurements.

1.4.3 Air Quality

Europe and other densely populated areas in the world are confronted with increasing levels of air pollution such as aerosol, nitrogen oxides, ground-level ozone, carbon monoxide, sulphates and other man made pollutants. Increased population, expansion of urban areas, increased traffic, and economic growth are the cause of the rising levels of air pollution. Carbon monoxide (CO), nitrogen oxides ($NOx=NO+NO_2$) and sulphur dioxide (SO_2) are primary pollutants emitted as a result of fossil fuel combustion. Sulphur dioxide is emitted by coal burning plants, nitrogen oxides primarily by road traffic, carbon monoxide primarily by bio-mass burning. Activated by sunlight, nitrogen oxides photo-chemically react with hydrocarbons or carbon monoxide to form ozone, a secondary pollutant. Oxidation of gas phase sulphur and nitrogen oxides leads to the formation of aerosol particles.

Usually, air pollution is divided into two main categories: Los Angeles type smog and London-type smog. Los Angeles-type smog arises when both sunlight intensity (UV radiation) and emissions from fossil-fuel combustion sources are high, i.e. in summertime when photochemical activity is high. "London-type smog" appears when both relative humidity and sulphur emissions from coal-fired power plants are high but sunlight is less intense, i.e. in autumn and wintertime. Many cities in Europe experience both types of smog. However, in many urban areas around the world, air pollution today is characterised more by the formation of ozone, other oxidants, and particles rather than by SO_2 and sulphuric acid. In these regions, the primary pollutants are aerosol, NO_x and volatile organic compounds.

Recently, long-range transport of pollutants has become a prominent issue as it affects background levels of air pollution that cannot be controlled by local measures. Already in the 1960's scientists demonstrated that sulphur emissions from continental Europe caused acidification of Scandinavian lakes. Also, it became apparent that Saharan dust transport events can bring substantial amounts of mineral dust from Africa to Europe. In April 2001, large quantities of mineral dust from Asian deserts where observed in the US throughout the atmospheric boundary layer with almost no reduction in concentration. The total amount was comparable to the daily emission flux of PM10 (particulate matter size 10 micron) from all US sources combined. Added to local air pollution, it elevated urban PM to levels that were exceeding health limits (EOS 84, 46, p.501, Nov 2003). These examples show that air pollution issues must be viewed on a global scale.

There is broad agreement that air pollution adversely affects human health. Approximately 1.3 billion people worldwide suffer from high levels of air pollution that according to the World Health Organisation (WHO) is unfit for consumption. High levels of aerosol, soot and other airborne particles are cause of respiratory disease. For example, particles emitted by diesel engines can induce respiratory tract allergies, in particular asthma. In general, allergies, skin diseases, immune system deficiencies are thought to be related to high levels of air pollution. Recently, it became known that cardiovascular disease can be induced by air pollution, mainly by particulate matter. The heart rate variability seems to be related to air quality [private communication MRC Institute for Environment and Health, Leicester, UK]. A recent study suggests that the level of traffic exposure at the residence of birth (elevated levels of CO and benzene) may explain a higher risk in schizophrenia (Atmospheric Environment 38, 2004, pp.3733-3734). In all these studies there is a need for data on real-time cumulative exposure to air pollution (particulate matter and gases) for specific groups of patients at their physical location over the study time period.

Policy on Air Quality

The United Nations Economic Commission for Europe (UN/ECE) Convention on Long-Range Trans-boundary Air Pollution (CLRTAP) (http://www.unece.org/env/lrtap_/lrtap_h1.htm) requires a consistent long-term monitoring programme for air pollution. Since its introduction in 1979 the convention has been ratified by almost all European countries, the Russian Federation, the USA and Canada. Following the convention the EC has introduced controls on emissions of sulphur, nitrous oxides (NOx), volatile organic compounds (VOCs), heavy metals, persistent organic pollutants

(POPs). The most recent Protocol (Gothenburg, 1999) introduces a multi-pollutant, multi-effect approach to reduce emissions of sulphur, NOx, VOCs and ammonia (NH_3), in order to abate acidification of lakes and soils, eutrophication, ground-level ozone, and to reduce the release in the atmosphere of toxic pollutants (heavy metals) and Persistent Organic Pollutants (POP).

It is stated in the Convention that monitoring of the concentrations of air pollutants is necessary in order to achieve the objectives. The Cooperative Programme for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe (EMEP) provides this information. Parties to the Convention monitor AQ at regional sites across Europe and submit data to EMEP. EMEP has three centres that coordinate these activities of which NILU is one. There are two large databases; the measurement database and the emission database. The AIRBASE database of the ETC/ACC forms the reference data set for the European ground-based observation network (6). In addition to measurements, EMEP maintains and develops an atmospheric dispersion model. The model calculates averages over a grid with a resolution of 50 km x 50 km. EMEP network density depends on the species measured, for NO_2 there are close to 100 sites, for VOC the number of measurement sites is less than 10. The required laboratory accuracy is 10 to 25%. At present 24 ECE countries participate in the EMEP programme (7).

The EU is strongly committed towards cleaner air and has introduced the Clean Air for Europe (CAFE) programme (http://europa.eu.int/comm/environment/air/cafe.htm). The objective of CAFE is to develop, collect and validate scientific information relating to the effects of outdoor air pollution, emission inventories, air quality assessment, emission and air quality projections, cost-effectiveness studies and integrated assessment modelling. This information is needed for development of air quality objectives and for the identification of measures required to reduce emissions (8).

The EC has introduced a series of Directives to control levels of certain pollutants and to monitor their concentrations in the air. In 1996, the Environment Council adopted Framework Directive 96/62/EC on ambient air quality assessment and management. This Directive covers the revision of previously existing legislation and the introduction of new air quality standards for previously unregulated air pollutants. The list of atmospheric pollutants to be considered includes sulphur dioxide, nitrogen dioxide, particulate matter, lead and ozone, benzene, carbon monoxide, poly-aromatic hydrocarbons (PAH), cadmium, arsenic, nickel and mercury (1-5).

Community-wide procedure for the exchange of information and data on ambient air quality in the European Community is established by the Council Decision 97/101/EC. The decision introduces a reciprocal exchange of information and data relating to the networks and stations set up in the Member States to measure air pollution and the air quality measurements taken by those stations (6).

The European Environmental Agency (EEA) is the European coordinating facility of the EC DG Environment. The EEA conducts the European State of the Environment assessments, the next one being planned for 2005. The actual work is carried out by a number of Topic Centres. Relevant here is the European Topic Centre on Air and Climate Change. The ETC/ACC consists of a consortium of 13 European institutes lead by RIVM. The products and services from the ETC/ACC on air pollution include the Report on Air Pollution in Europe containing trends and appraisal of current policies, CLRTAP emission inventory, maintenance of the air quality information system AIRBASE and support to the CAFE programme (7). It will also develop information systems on air quality and emissions via Internet.

Besides international directives and convention, each state and region has to its own policy, limit values and monitoring standards for air pollution. However, international standards are gradually taking over, allowing a more uniform approach to the problem.

***Major environmental treaties and Council Directives on Air Quality*:**

(1) Council Directive 96/62/EC on ambient air quality assessment and management.
(2) Council Directive 1999/30/EC on limit values for SO_2, NOx, particulate matter and Pb in ambient air. Revised by decision 2001/744/EC (OJ L 278/35)
(3) Directive 2000/69/EC on CO and benzene.
(4) Directive 2001/81/EC on national emission ceilings for SO_2, NOx, VOC and NH_3 attained by 2010
(5) Directive 2002/69/EC of the European Parliament and of the Council relating to ozone in ambient air and ceilings on atmospheric pollutants. (OJ L 67/14).
(6) Commission Decision 97/101/EC on reciprocal exchange of information and data from networks and individual stations measuring ambient air pollution within the Member States 2001/752/EC.
(7) Commission Decision 2001/839/EC of Nov 2001 laying down a questionnaire for annual reporting on ambient air quality under Council Directives 96/62/EC and 1999/30/EC (OJ L 319/45)
(8) Clean Air For Europe (CAFE) programme, COM(2001)245 of 4.5.2001

Air Quality Observations

Monitoring air quality is mostly performed using ground-based, in-situ measurements. This has the advantage of being accurate and reliable and to measure at the place of risk, i.e. at human nose level. Also, the limit values for air pollutants are often given in terms of quantities that are obtained from in-situ instruments. However, information on the spatial distribution (horizontal, but also vertical) and transport of atmospheric pollutants is often limited. This information can be supplemented by remote sensing information from ground, airborne, and space instruments. In particular, long-range transport of pollutants that establishes a background to concentration levels caused by local emissions, could be supplied by satellite remote sensing.

However, to date, satellite measurements are seldom used for the monitoring of air pollution. This is so because the retrieval of information from the planetary boundary layer from space is difficult and often impossible because of the presence of clouds. Satellites instruments operating in nadir mode usually provide trace gas total columns integrated from the surface to the top of the atmosphere, which contains the total troposphere and stratospheric amount. For some gases (limited) profile information may be retrieved from the spectral properties through their dependence on temperature and pressure subsequently linked to altitude in the atmosphere. For ozone limited profile information can be obtained in nadir observation from the Huggins band which varies with temperature. Satellites equipped with limb and occultation observation mode provide good vertical resolution but do not reach down to the planetary boundary layer. For other AQ constituents such as NO_2, CO, SO_2 and aerosol, obtaining height resolved information from satellite measurements requires more subtle tricks.

In recent years it has been shown that for a limited number of trace gasses it is possible to estimate the tropospheric column, notably nitrogen dioxide, carbon monoxide and ozone. These estimates use a combination of clouded and cloud-free scenes, combine different satellites with different views, use model information from data assimilation, or take advantage of the altitude information contained in the pressure broadening of molecular lines in the mid-infrared. Maps thus obtained of tropospheric trace gas columns provide unique information on the spatial distribution of pollutants on a regional and continental scale. For example, recent NO_2 maps obtained from SCIAMACHY measurements show in great detail the European polluted areas and their cross boundary transport. Global maps of CO produced by MOPITT have revealed important processes in emissions and transport of industrial and biomass burning events.

Aerosol retrieval from satellites is a challenging task, due to their highly variable spatial and temporal concentration distribution and the fact that additional parameters are required to characterise aerosol scattering and absorption features being determined by their chemical composition and size distribution. Size distribution is classified in PM10 (particulate matter of diameter <10 micron), and PM 2.5 (<2.5 micron). Discussion are taking place to introduce PM1 (<1 micron) as a requirement for air pollution for its significant impact on health. In aerosol retrieval usually a number of assumptions on the above parameters are made. The most common satellite aerosol product is total aerosol optical depth. Satellite instruments with multiple views (ATSR-2) and/or detection of the polarization state of the radiation (POLDER) provide more and better information on aerosol, exploiting the characteristic features of phase function and polarisation to characterise the scattering particle and its location. Additional information on the proportion between scattering and absorption of the aerosol is obtained from the single scattering albedo. This information is important for climate applications but also to characterise the type (and size) of aerosol.

The temporal resolution of present generation satellite systems is not good enough to meet requirements; most air pollutants show strong diurnal variation, which is not captured by polar orbiting satellites. Also, boundary layer measurements can only be made under cloud-free conditions. This introduces selection effects such that these measurements may not be representative for longer-term (e.g. daily, monthly and annual) average values. Recently, atmospheric chemistry missions in geo-stationary orbit have been proposed both in Europe and the USA [RD11]. From geo-stationary orbit the diurnal changes of pollutants can be followed during the day. This would be an important step forward in the utilization of space based instruments for air pollution monitoring.

The most promising route for satellite measurements to reach their potential contribution to air pollution monitoring and forecasting, is through data assimilation and modelling of both satellite and ground based in-situ measurements into an atmospheric chemistry transport model. This is the route taken here by the CAPACITY project.

Integration of Air Quality data into Models

Chemical transport models are increasingly applied to provide air quality information. The models are fed by meteorological fields, contain emission databases and take chemical conversions and deposition into account. Data assimilation is used to improve the models by taking measurements into account. The use of models also allows the construction of air pollution forecasts through forecast meteorological fields, sometimes called chemical weather forecasts. Examples are the EURAD forecast model system, developed at the Rheinish Environmental Institute of the University of Cologne and the CHIMERE model used for the air pollution forecast for France (http://prevair.ineris.fr). The global MOCAGE model of Meteo-France also has the ability to zoom in on local scale. Presently many Meteorological institutes including ECMWF have started activities in the field of chemical weather forecast.

The well-tested EURAD forecast system consists of three major components: The PennState/NCAR mesoscale model MM5 to predict the needed meteorological variables, the EURAD Emission Module (EEM) to calculate the temporal and spatial distribution of the emission rates of the major pollutants and the EURAD Chemistry Transport Model (EURAD-CTM) to predict the concentrations and deposition of the main atmospheric pollutants. More then 60 reactive species and an aerosol model are included in this model. The model system is using the method of nested simulations. This enables consistent modelling of air quality from small (local) to large (continental) scales. The model system has been applied to the assessment of emission changes as a contribution to the development of strategies for the reduction of air pollution levels in Europe. At this point in time satellite data have been assimilated in experimental mode.

The CHIMERE model covers Western Europe at a 0.5° horizontal resolution. Five vertical layers cover the lower troposphere up to 700 hPa (~3 km). Several nested domains with a 4-6 km horizontal resolution are implemented for several French agglomerations (Paris, Marseille, Strasbourg and Lyon area). The continental and the nested model are forced by forecast meteorological fields delivered by ECMWF every 3 hours. All relevant physical processes concerning advection, vertical mixing, radiation attenuation by clouds, dry deposition, etc. are included in the model. Annual gaseous species emissions (NOx, CO, VOC, SO2, NH3) are taken from EMEP, VOC and temporal profiles are provided by University of Stuttgart. Bio-genic isoprene, terpene and NO emissions are included.

Climatologically monthly average boundary conditions are taken from the global scale chemistry-transport model MOZART. Initial experiments with satellite data assimilation in CHIMERE show that forecast quality is improved.

On a more detailed scale, useful to cities and urban areas, dispersion models with prescribed emissions are in use. Chemical effects are accounted for by including (photo) chemical reaction schemes including tropospheric ozone, NOx, sulfates and Carbon bond mechanisms. An example is the ADMS-Urban model developed by Cambridge Environmental Research Consultants Ltd. The model contains hundreds of pollutant emission sources from industry, traffic and other sources to allow the accurate forecasting of street level air quality. Whilst such models are able to accurately describe the effect of local emissions they rely on the input of regional air pollution data to provide for background air pollution data outside the modelled area. These additional data may be supplied by regional or cross boundary stations if available. Usually, regional scale CTM generate the boundary conditions to the urban scale model. Thus a nested set of models is created, going from global to regional to local models.

1.4.3.1 Air Quality Requirements

Air Quality requirements are driven by the need to probe the planetary boundary layer (PBL) at high horizontal and temporal resolution. Daily, even hourly time resolution is required to capture the diurnal variation of atmospheric constituents involved in air quality (CO, aerosol, troposphere ozone, SO_2 etc). Horizontal contiguous sampling at km scale is required in order to capture the localised emission sources in urban areas. In order to capture long-range transport of air pollutants it is also necessary to carry out observations of the free troposphere (FT) adjacent to the PBL. Satellites can provide input to the observational capacity by continental scale coverage and area averages of pollutants, notably NO_2 and aerosol.

Traditionally, the requirements for AQ monitoring are grafted on the means available for verification and enforcement, which is the ground based network at local and regional authority level. These data are often of limited use in a global observation system, through lack of standardisation of instruments and data produced. Continental and hemi-spherical coverage cannot practically be covered by the ground-based measuring network. On the other hand, satellite measurements are not expected to be of sufficient resolution and quality to contribute information on air quality at local ground level. Therefore, a synthesis of data and model information must be found. We adopt here the approach of an Integrated Observation System for air quality monitoring and forecast [RD1] combining satellite data, surface data, aircraft and balloon data with models through data assimilation. Inverse modelling will be needed to derive emissions. Campaigns are necessary for process studies needed for scientific understanding. In the following requirements are defined at system level.

In the following requirements will be based on requirements developed earlier and laid down in the documents IGACO [RD1], the GMES-GATO report [RD2], the EUMETSAT position paper on short range forecasting [RD4], the ICAO Manual on volcanic ash, radioactive material and toxic clouds [RD6], the WMO/CEOS GAW report [RD7], and the EUMETSAT requirements for Geo-stationary satellite observations [RD9]. Additional information is obtained from the ESA Earth Explorer proposals GeoTROPE [RD11] and TROC [RD 12]. These findings are critically reviewed and adapted to meet new insights as formulated during the User Consultation meeting 20-21 January 2004 at ESTEC. A distinction is made between threshold requirements (minimum requirement to satisfy some user needs) and target requirement (optimum requirement to satisfy most user needs).

Air Quality Monitoring

The driving requirements are set by the EU framework directives on ambient air quality for surface concentration levels of regulated compounds O_3, SO_2, NO_x, PM10, PM2.5, CO, benzene (C6H6), Poly Aromatic Hydrocarbons (PAH), Pb, Ni, As, Cd, Hg. Requirements on emissions are set by the National Emission Ceiling Directive for SO_2, NO_x, VOC, NH_3 and fine particulate matter.
The CLRTAP convention sets emission ceilings on SO_2, NO_x, VOCs, NH_3.

Emissions from ships requiring measurement over coastal waters was added as a requirement during the user consultation meeting and includes CO emission, see also the GMES-GATO report [RD2].
Formaldehyde (HCHO) is considered an important indicator species for photochemical oxidising activity in the PBL.

Long term monitoring should extend over at least two solar cycles, i.e. a time period of about 25 years. The required coverage is continental, but global coverage is desired. Observational requirements for short range forecasting formulated by EUMETSAT [RD4] are most challenging but considered appropriate for the specification of a future atmospheric chemistry monitoring mission becoming operational in the 2015-2025 era. These requirements agree with requirements derived in the EUMETSAT study on Geo-stationary Satellite Observations for Monitoring Atmospheric Composition and Chemistry applications [RD 9].
Day time measurements are required, night time measurements are desirable. Horizontal resolution for measurements of O_3, CO, SO_2, NO, NO_2, HCHO, PAN, VOC is: threshold 10 km and optimum 2 km. Vertical resolution requirements are: threshold tropospheric column and optimum 2 km. Temporal resolution is: threshold 2 hrs, optimum 30 minutes. Accuracy threshold 50%, optimum 20%, except for O_3 and CO which should have threshold 10% and optimum 5% accuracy.
For aerosol requirements are formulated for optical depth, size distribution, and single scattering albedo. Horizontal resolution ranges from threshold 5 km to target 0.5 km. Vertical resolution ranges from threshold total column to target tropospheric column and boundary layer (2 pieces of information). Temporal resolution is: 1 hrs threshold and 15 min target. Accuracy threshold 5%, target 1%, except for size threshold 30%, target 10%.
A number of ancillary parameters are also required. These include temperature profile, cloud cover, humidity profile, lightning location and fire location. Similar spatial-temporal specifications apply as for gases and aerosol. In addition requirements for surface UV-A and UV-B apply, as already specified with the surface UV requirements.

Air Quality Forecasting

The main driver is the requirement for predicting air pollution levels arising from industrial activity (energy and transport) on regional and local scale and issuing warnings when limit values will be exceeded. Natural hazards such as volcanic eruption, forest fires and man made hazards such as chemical and nuclear releases are based on dispersion model forecast that are fed by observations. Requirements are formulated in the EUMETSAT short range forecasting position paper [RD4] and in the Manual on Volcanic ash, radioactive material and toxic chemical clouds from the International Civil Aviation Organisation [RD6]. Volcanic eruption requirements are elaborated in the GMES-GATO report [RD2,Ch5]. The delay time allowed for data delivery of above atmospheric constituents is typically 30 min threshold to 15 min target value. Source detection and attribution of the emissions of aerosol and precursors such as SO_2, NO_2 and secondary organic compounds is an important requirement for a health and safety forecast system.

For forecasting the same requirements apply as for monitoring except for the delay time in providing the observational data which is an additional requirement.

Understanding of Air Quality

Issues to be addressed include the oxidising capacity of the atmosphere, the long-term trend in tropospheric ozone and the long-range transport of pollutants.
The oxidising capacity of the atmosphere is governed mainly by OH. The trend in OH needs to be known to better than 1% global average, regionally better than 5%. An integrated quantity (weighted by CH_4 removal) is needed. Indirect methods available include the measurement of methyl chloroform. More direct methods are the simultaneous measurements of H_2O, O_3, NO_x, CH_4 and CO in combination with modelling.
Analysis of causes of OH change require requires observational data at process level:

- Production: O_3, NO + NO_2, H_2O_2, ROOH, photolysis rates, temperature and humidity profile
- Loss: CO, CH_4, Hydrocarbons, CH_2O, O_3, NO_2, and others

Related data: HO_2, CH_3O_2,
Relevant Scales: see IGACO [RD1]

Modelling is needed on:

- Emissions (NO_x, Biomass Burning)
- Surface Albedo, J-values, Aerosols.

The trend of tropospheric ozone requires accurate monitoring (10% threshold, 5% target) of ozone concentrations as well as precursor gases NO_2 and CO. Analysis of causes requires additional data on:

- understanding deposition:
- Stratosphere/Troposphere Exchange
- Photolysis Rates + Temperature
- Hydrocarbons (VOC, natural) CO, CH_4, H_2O, NO_x (NO + NO_2), CH_2O, PAN

Long Range Transport of pollutants requires global observations on: CO, NO_x/NO_y, O_3, PM10/2.5/1, POPs, Hg at horizontal resolution 10 km down to 3 km and vertical resolution FT/BL/UTLS partial columns down to 2 km. Temporal resolution: 1 hr down to 30 min (fronts).

1.4.3.2 Air Quality Services

Air Quality services are developed in consultation with the following user organisations involved in he ESA GMES Service for Atmosphere:

- EEA directly and through the TC ACC members RIVM and NILU
- EMEP (NILU)
- EMPA (Swiss Environmental Agency
- EPA (Irish Environmental Protection Agency)
- LUA (Rheinland-Westfalen Environmental Agency)
- ADEME (French national environmental measurement network agency)
- INERIS (French national coordinating environmental agency)
- AirParif (Paris Air Quality agency)
- UBA-A (Austrian Environmental Agency)
- JRC-IES (European Joint Research Centre Institute for Environment and Sustainability)
- ARPA (Air quality agency Lombardia and Emilio-Romagna)

AQ monitoring

Primary products for AQ Protocol Monitoring:

a. PBL and FT NO2 global field, location specific time series
b. PBL and FT O3 global field, location specific time series
c. PBL and FT aerosol AOD/Å, regional/global time series, annual mean
d. FT SO2, high pollution regions/episodes
e. FT HCHO, high pollution regions/episodes
f. PBL and FT CO total, regional, global
g. PBL and FT CH_4 total, regional, global
h. PBL and FT H_2O vapour, regional and global

AQ forecast

Primary product for AQ Forecast:

(a) Air Quality Forecast regional, local.

(b) Air Quality Index based on mixture of O_3, NO_2, PM10, SO_2, and CO ground level values, accuracy according to EC directives.

AQ Understanding

Primary product for Understanding (accuracy):
A similar list of products applies as for AQ monitoring. In addition, the oxidising capacity of the atmosphere requires the free troposphere to be included in the requirement specification. The global nature of long-range transport requires global coverage. The downward transport of ozone requires the UTLS region to be included in the specification.

1.4.4 Climate Change

Systematic and continuous observation of climate parameters is necessary in order to understand and predict climate variability and change caused by human activities (IPCC, 2001). This includes the monitoring of physical parameters of the atmosphere, ocean and land. For the atmosphere part of System Earth, this involves the monitoring of emissions and concentration distributions of greenhouse gases and aerosol. The most important greenhouse gases are CO_2, CH_4, tropospheric O_3, N_2O, and CFCs. Aerosols can be either emitted directly, e.g. in the form of soot, or formed indirectly in the atmosphere from emitted gaseous precursors such as SO_x, NO_x and NH_x.

Kyoto Protocol

The UN Framework Convention on Climate Change (UNFCCC) adopted at the Earth Summit of Rio de Janeiro in 1992 and the resulting Kyoto Protocol (1997) commits signatories to cut the emissions of greenhouse gases by 8% in the 5-year period 2008-2012 compared with 1990 levels. The Kyoto Protocol confines itself to the emission of six main greenhouse gases, CO_2, CH_4, N_2O, HFC's, PFC's and SF_6. The European Community ratified the Kyoto Protocol on 31 May 2002 following Commission Decision 2002/358/EC.

The Kyoto Protocol is legally regulated in the EU by the Council decision 93/389/EEC for a monitoring mechanism of Community CO_2 and other greenhouse gas emissions and its amendment (Council Decision 99/296/EC). These decisions establish a mechanism designed to monitor all anthropogenic greenhouse gas emissions not controlled under the Montreal Protocol and its Amendments and evaluate progress made in this field to ensure compliance with the Community's commitments concerning climate change.

In the evaluation of these Decisions (1999/296/EC) the progress towards reduction is assessed. Projections indicate that existing measures will not be sufficient to reach reduced emission goals for 2008-2012. To close this gap the ECCP (European Climate Change Programme) was initiated.

The European Climate Change Programme and a number of Council and Commission decisions stress the need for monitoring GHG emissions and sinks as a means for assessment of progress toward meeting Kyoto Protocol targets. There is a decision for a new monitoring mechanism recently ratified by Parliament, which replaces the former decisions. It reflects the guidelines from the UNFCCC as newly set out in Bonn and Marrakech (COP 6 and 7), and provides further harmonization of emission forecasts and addresses requirements relating to ratification of the Kyoto Protocol and the burden-sharing between the Community and its member states.

Global greenhouse gas emissions and absorptions, sources and sinks, are not well known. There is a large discrepancy between bottom-up emission estimates, derived from national government energy, transport, agricultural, etc figures, and top-down estimates derived from atmosphere concentration distributions. Better source and sink estimates are needed to support the Kyoto Protocol monitoring, verification and reporting obligations. To date, no independent global observation system for the monitoring of GHG emissions exists. This seriously limits the (independent) verification of Protocol targets.

Climate Observations

Global distributions of greenhouse gases need to be monitored in the free troposphere where radiative forcing is strongest. The monitoring of emissions requires probing the planetary boundary layer. The global scale of the protocol-monitoring requirement dictates the use of satellites as the only means of getting global coverage at reasonable spatial and temporal resolution and in a cost effective manner. Continuity in satellite observations is necessary in order to establish long term monitoring series (trends). Improved monitoring methods need to be based on integration of surface data and space data into models, similar to the approach advocated by IGACO. In combination, useful information is expected to become available for end-users.

The retrieval of total columns of GHG from satellites is a relatively new development in satellite remote sensing. The NASDA ADEOS-1 satellite carrying the IMG instrument was the first to achieve global coverage of GHG total column measurement, owing to its polar orbiting satellite and a nadir-viewing instrument. Due to satellite failure this measurement series was prematurely aborted (1996-1997). The NASA polar orbiting EOS Terra (1999-present) carrying the nadir viewing MOPITT instrument allows total column measurement of CO and CH_4. Due to instrument problems, methane data are not available. The ESA ENVISAT (2002-present) carrying SCIAMACHY (nadir and limb) and MIPAS (limb) are capable of measuring a range of GHG. The NASA EOS Aqua satellite (2002-present) carries the AIRS instrument with CO_2 measurement capability. The NASDA ADEOS-2 (2002-2003) carries the ILAS-II occultation instrument with GHG measurement capability at limited global coverage, but has recently ceased operation due to satellite failure.

The NASA EOS Aura satellite (2004-2010) will provide new GHG measurement capabilities with the nadir-limb viewing TES instrument on board. Limb viewing HRDLS may provide additional information. Subsequently, the OCO satellite planned in the NASA ESSP-3 programme will provide a more powerful carbon dioxide measurement facility. On the Japanese side the ADEOS-3 (2007) with ILAS-II on board and GCOM (2007) with a to be defined payload will be of interest to GHG measurement. Long-term monitoring of GHG distributions will be achieved to some extent by the EUMETSAT MetOp series (2005-2020) with the nadir viewing instrument IASI.

The measurements of ENVISAT, particularly the instruments SCIAMACHY and MIPAS are expected to provide improved greenhouse and related gas distributions and emission inventories for the period 2002 to 2007 and possibly beyond. Improvements will be achieved through a combination of advanced data retrieval, data assimilation and (inverse) modelling. It is expected that improved global emission estimates of methane, carbon monoxide and possibly carbon dioxide will become available. The global column distribution of other greenhouse (N_2O) and related gases (NO_2, SO_2) will be monitored.

Climate Models

Using accurate trace gas measurements, emission estimates can be derived using inverse modelling. These techniques have been developed and applied successfully in the past on a number of trace gases including CO_2 , CH_4 and CO. The EU project EVERGREEN currently develops the inverse modelling of these gases based on ENVISAT satellite measurements [RD15]. Three ACT models are being considered: the TM3 model at KNMI, the TM5 model at JRC-IES, the TM derivative of the Max Planck Institute for Bio-Geochemistry and the IMAGE model at IASB. A model inter-comparison exercise is currently underway comparing (vertical) transport of these models with tracer gases and comparing the chemistry module with a fixed initial OH field with measured distributions of methyl chloroform. Some models are driven by ECMWF fields, others calculate the average monthly concentrations. A combined inverse modelling and assimilation technique is used, based on variational (4D-Var) data assimilation. Models will be constrained by measured normalised vertical columns. The main input data are ENVISAT-SCIAMACHY vertical columns of the gasses CO, CO_2 and CH_4.

The above project has made clear that a high accuracy and a high spatial and temporal resolution is required in order to constrain the models by observation. Measurement accuracies at the percentage level or better need to be achieved in order to be of value. For some greenhouse gases CO_2, O_3 and precursor gases CO (precursor to CO_2), NO_2 (precursor to tropospheric O_3), SO_2 (precursor to aerosol) a temporal resolution of a few hours is needed due to the diurnal variation of these gases. Recently, comparison of SCIAMACHY methane measurements with models have shown good overall agreement, but interesting differences are revealed near the tropics. These have been attributed to hitherto unaccounted for methane emissions. Thus, the potential to improve emission inventories by top-down measurement of GHG distributions has been demonstrated.

1.4.4.1 Climate Requirements

Requirements are driven by the need to accurately monitor trends and variability of atmospheric climate parameters. For radiative forcing the main domain of interest is the UTLS where radiatively active gases need to be measured at relatively high vertical resolution. Also aerosol and cloud parameters need to be observed in the UTLS region at less stringent vertical resolution. Requirements have been formulated for the ACECHEM mission specification [RD10]. The requirements pertaining to climate constituents are considered suitable for the UTLS component of an operational Atmospheric Composition monitoring mission.

For climate emissions the area of interest is the PBL and free troposphere. Requirements respond to the Kyoto Protocol. They are driven by the very high accuracy required of concentration differences measurement of greenhouse gases and aerosol. The coverage of the observations is global but needs to be projected down to regional and local scales. The time span of observations is several decades and thus demand on accuracy and homogeneity of successive data series is high.

Understanding climate change requirements are driven by long-term climate-chemistry interactions. This requirement includes understanding of the anthropogenic versus natural component of emissions and sinks, the interaction between radiation, dynamics and composition, including the oxidising capacity of the troposphere, the increase in stratospheric water vapour and the interaction of climate and stratospheric ozone.

Climate research is often carried out at meteorological centres that rely on Numerical Weather Prediction models. In order to improve climate monitoring there is a technical advantage by including atmospheric composition observations Near Real Time in the operational assimilation system of NWP centres. In this case near-real time data delivery would become a requirement.

The Implementation Plan for the Integrated Global Observing Systems for Climate (IGOS-C) in support of the UNFCCC [RD8] defines Essential Climate Variables (ECV) to fulfil the observation requirements that are required by the Parties to the UNFCCC (Decision 11/CP.9 of the Conference of Parties). The implementation plan builds on the GCOS Second Adequacy Report, earlier reviewed by the Scientific and Technological Advice body of the COP (June 2003). The atmospheric composition observing network is largely based on the WMO GAW network [RD7]. The ECV's in the higher layers of the atmosphere are, according to GCOS, adequately covered by the Global Upper Air Network (GUAN). Requirements for H_2O, CO_2, CH_4 and other GHG, O_3 and aerosol are given, based on the various ground based monitoring and flask sampling networks (see Chapter 2.4) supplemented by satellite measurements (SCIAMACHY, AIRS for GHG and AVHRR, MODIS, AIRS for aerosol). The GCOS implementation plan falls short in its observation requirements for the stratosphere and the upper troposphere which is not given. The list of atmospheric composition gases does not include the precursor gases (CO, NO_x, SO_2). Accuracies quoted do not permit the derivation of sufficiently accurate emissions by inverse modelling techniques.

Requirements for the retrieval of emissions of GHG from direct observations, as opposed to country wise bottom up accounting, are more demanding in accuracy than the trend and variability requirements discussed above. Owing to the long lifetime of GHG, compared with tropospheric mixing times, the concentration distribution is almost uniform. Small variations in the concentration distribution of CO_2, CH_4 however may allow the retrieval of emission rates. This possibility is currently explored in the EU 5FP project EVERGREEN [RD15]. Notably, ENVISAT satellite measurements in combination with model data are expected to yield improved methane emission data. The ESA study on the potential of space borne remote sensing to contribute to the quantification of anthropogenic emissions in the frame of the Kyoto Protocol [RD3], proposes requirements on accuracy and on spatial and temporal scale for GHG emission retrieval. These requirements are demanding for satellite observations. For Kyoto Protocol monitoring, emissions at percentage level accuracy are required which leads to much higher accuracy (better than 1%) in total column measurements.

For the purpose of this requirement specification the requirements laid down in the IGACO report [RD1] are regarded as most appropriate. These requirements are more demanding than the EUMETSAT requirements on short range forecasting and geo-stationary satellite observations [RD4 and RD9]. Target IGACO requirements are consistent with the ESA Kyoto study [RD3]. Present requirements would fall short in meeting the source attribution and emission strength requirements for CO2 and N2O set by the Kyoto Protocol. However, currently global emission inventories are mostly based on models rather than measurements. Current progress in inverse modelling indicates that improvements in the emission inventories are possible with the requirement specifications presented here.

Treaty monitoring and Verification

The main drivers are the UNFCCC and the resulting Kyoto Protocol. Monitoring of concentration distributions and inverse modelling of emission of GHG gases, precursor gases and aerosol are required.

The IGACO [RD1] requirements distinguish between partial column measurements of lower troposphere LT, upper troposphere UT, lower stratosphere LS, upper stratosphere US and troposphere column TC, in addition to total column measurements. Requirements for CO_2 and CH_4 are typically horizontal resolution 50 km threshold and 10 km target in the lower troposphere, 50 km (250 km) higher up in the atmosphere. The vertical resolution for CO_2 is 0.5 km target, 2 km threshold in the lower troposphere relaxing to 2 (4) km higher in the atmosphere. The temporal resolution is 3 hrs (target) to 12 hours (threshold) in order to capture diurnal variation of CO_2. This requirement deviates from IGACO where a 6 hrs target and 3 day threshold requirement has been given. The precision(accuracy) depends on the species. For CO_2 this is 0.2(1)% target in the LT increasing to 1(2)% higher in the atmosphere. For CH_4 precision(accuracy) requirements are LT 1(2)% relaxing to 2(5)% higher in the atmosphere. For the GHG precursor gases and for aerosol the same requirements apply as to AQ.

Climate Predictions

For climate simulations a number of species are required to be measured in the PBL including aerosol, H_2O, CO_2 and O_3. In the free troposphere the H2O profile is required, together with columns of tropospheric ozone, aerosol and cirrus (AOD). For reanalysis of previous and analysis of current climate conditions the assimilation of satellite observations in models is required.

Climate prediction models need to be validated by measurement of relevant climate parameters. Confidence in the predictive capability of models is gained by simulation of the recent past captured by monitoring measurements.

Understanding of Climate Change

The radiative forcing and its change needs to be understood. Also the effect of spatial distribution to local climate needs to be investigated. In particular the role of aerosol in radiative forcing and its diurnal variation needs to be understood. Requirements are similar as under monitoring. The role of the Brewer Dobson circulation on climate and changes in this circulation need to be monitored by tracer gases (CH_4, N_20, CO, HCl) and meteorological parameters. The position and strength of the polar vortex needs to be monitored. The position and strength of the inter tropical conversion zone (ITCZ) needs to be measured.

The underlying processes in climate-chemistry interaction need to be understood. A good review of climate chemistry interaction can be found in the report of the joint SPARC/IGAC workshop in Giens, France, 3-5 April 2003 [RD 18]. Observation requirements for stratosphere-troposphere coupling, lower stratosphere and troposphere ozone, aerosol and water vapour have been formulated.

Requirements include measurement of atmospheric constituents in the Upper Troposphere-Lower Stratosphere (UTLS) layer that are both chemically and radiatively active, such as H2O, O3, aerosol and clouds. Common tracers such as N_2O, CH_4, CO and HCl can reveal ozone transport processes across the tropopause. The trend in (lower) stratospheric H_2O needs to be measured at 1% accuracy.

Tropospheric aerosol requires special attention for its uncertainty in current climate models. This uncertainty is due to their highly variable nature in space and time. The magnitude of aerosol forcing is comparable to gaseous forcing but of opposite sign. However, due to the local/regional nature, variable vertical distribution and the strong diurnal variation no simple conclusion is possible. High spatial and high temporal resolution concentration distribution measurements are required. Additional parameters are needed to fully characterise the scattering and absorbing properties of aerosol. These include single scattering albedo and phase function providing information on the absorbing properties of the aerosol and information on size and shape. The fact that from space there are no direct measurements but retrieved properties requires additional in-situ measurements to fully characterise the aerosol. Furthermore, connecting emissions of aerosol and gaseous precursors to spatio-temporal distributions of aerosol requires information on aerosol transport, transformation and their interaction with clouds.

The role of changes in the oxidising capacity of the troposphere in climate change needs to be understood. Additional species that are implied in these reaction cycles are CO, HNO_3, NO_x. Requirements are similar to those formulated under air quality understanding.

There are a number of other indicators of climate change and climate-chemistry interaction that need to be measured. These include aerosol absorption and scattering in the PBL as an indicator for surface temperature, clouds and aerosol in the troposphere, albedo measurements and aerosol over ice surfaces, measurement of dimethylsulfide (DMS).

1.4.4.2 Climate Services

Climate services are developed in consultation with the following user organisations involved in he ESA GMES Service for Atmosphere:

- NILU (emission database)
- UBA-A (Protocol monitoring)
- EPA (Protocol monitoring)
- JRC-IES (inverse modelling of emissions)
- RIVM (emission database)

Atmospheric Composition Climate Monitoring

Primary products for Protocol Monitoring:

a. CH_4 global distributions time series
b. NO_2 global distributions time series
c. Tropospheric O_3 global distribution time series
d. Aerosol global distributions, single scattering albedo/phase function time series
e. CO global distributions time series
f. CO_2 global distributions time series
g. N_2O global distributions time series
h. H_2O global and regional time series
i. Spectral solar irradiance time series

Emissions of Greenhouse gases and aerosol

Primary products for Protocol Monitoring:

a. CO_2 global emissions
b. CH_4 global emissions

c. N_2O global emissions
d. CO global emissions
e. NO_2 global emissions
f. Aerosol global emissions

Understanding of Climate Change

Primary products for Climate Change assessment, notably climate-chemistry interaction

a. Tropospheric O_3 global distribution time series, UTLS at high vertical resolution
b. H_2O global and regional time series, UTLS at high vertical resolution
c. Aerosol global distributions, single scattering albedo/phase function time series
d. CH_4 global distributions time series
e. N_2O global distributions time series
f. NO_2 global distributions time series
g. HCl global distribution time series
h. CO global distributions time series
i. CO_2 global distributions time series

Spectral solar irradiance time series

2 Geophysical Data Requirements

2.1 Introduction

2.1.1 Purpose

This document, together with the Appendix 'Geophysical Data Requirements Tables', sets out the Geophysical Data Requirements for an Operational Atmospheric Chemistry Monitoring Mission. Operational in the sense that a reliable service of specified information can be established that satisfies user needs. Monitoring in the sense that a long-term continuity and consistency of the quality of the information can be achieved.

In Chapter 1 the user requirements have been defined at high level, identifying areas of application, needs for information, 'level-4' data requirements on spatial, temporal resolution and accuracy and other general requirements on timeliness and long-term continuity.

Following the logic of the CAPACITY project [AD1], in this Chapter the 'level-2' requirements on geophysical data products are derived from the user requirements for each of the applications. We set data requirements on individual (retrieved) products as these can be assessed quantitatively and used afterwards to drive instrument concepts.

The geophysical data has been divided into three categories:

- Satelliteborne level-2 atmospheric composition observations (retrieved products)
- Ground-based atmospheric composition observations (containing both level-2 retrieved products and in-situ observations)
- Auxiliary data: (Assimilated) model data, satelliteborne or ground-based data other than derived from atmospheric composition observations

2.1.2 Scope

'Capacity' is based on the vision, expressed in the IGOS/IGACO theme report [RD1], that user requirements for atmospheric composition monitoring can only be fulfilled by adopting an integrated approach to the global observation system by combining observations from satellite, ground-based, and airborne systems into numerical atmospheric (chemistry-transport) models in order to obtain a self-consistent and comprehensive description of the atmospheric composition.

In order to derive data requirements (level-2) based on given user requirements (typically level-4) first the respective role of satellite observations, ground-based observations and other auxiliary data sources needs to be assessed. Once these roles have been identified it is possible to derive a strategy for each of the applications on what are the atmospheric composition level-2 data requirements for operational satelliteborne observations, operational ground-based observations and, further, what are the auxiliary data requirements, including (assimilated) model data as well as data from observations other than atmospheric composition.

It should be clear that in the definition of the strategy several expert judgements have been made on the required level-2 products to arrive at the user requirements (typically level 4, sometimes also level 2 or 3). These judgements are, at least, partly based on current insights in retrieval practices and general capabilities of satellite sensors. For example, it was not considered useful to include requirements on compounds that cannot be observed from space from first principles, e.g., because relevant spectroscopic features are missing.

On the other hand, as few as possible compromises have been made in the translation of user requirements into data requirements to prevent early selections solely based on current practices that may be altered. As a result some of the given level-2 data requirements may be judged unrealistic stringent from an observational point of view. By iterations with WP2200 a balance is sought between data requirements that may be based on unrealistic user wishes and practical capabilities of current, planned and potential operational measurements.

The specification of data requirements in this document builds on the heritage from several (scientific) studies performed in the past. The ESA proposals for the Earth Explorer mission ACECHEM [RD10], GeoTrope [RD11], TROC [RD12], and the ESA study for greenhouse gas emission retrieval from space based measurements [RD 3] provide data requirements in different levels of detail. Also the EUMETSAT position paper on Observation requirements for Now Casting and Very Short Range Forecasting in 2015-2025 [RD4] and the EUMETSAT study for Geo-stationary Satellite Observations for Monitoring Atmospheric Composition and Chemistry Applications in 2015-2025 [RD9] established sets of requirements on the envisioned observations.

This document also draws on the work that is laid down in the IGACO theme report, approved by the IGOS-Partnership in 2004 [RD1]. That report in turn draws on requirement specifications developed earlier for the WMO GAW Programme [RD7]. Finally, this document has been completed in parallel to the initial phase of the ESA project for the GMES Service Element Atmosphere, PROMOTE that started in 2004, and to the preparatory phase of the EU GMES project GEMS.

2.1.3 References

Applicable Documents

[AD3] ESA ITT AO/1-4273/02/NL/GS of 7 November 2002, including Statement of Work EOP-FS/0647 of 25 July 2002

Reference Documents

[RD4] The Changing Atmosphere. The IGACO Theme report. Editors Leonard A Barrie, Peter Borrell, Joerg Langen, approved at IGOS-P meeting May 2004.

[RD2] GMES-GATO Strategy Report. Global Monitoring for Environment and Security-Global ATmospheric Observations. www.nilu.no/gmes-gato/download. March 2004.

[RD4] EUMETSAT position paper on Observation Requirements for Now Casting and Very Short Range Forecasting in 2015-2025. B W Golding, S Senesi, K. Browning, B Bizzarri, W Benesch, D Rosenfeld, V Levizzani, H Roesli, U Platt, T E Nordeng, J T Carmona, P Ambrosetti, P Pagano, M Kurz. VII.02 05/12/2003, 28 February 2003.

[RD6] WMO/CEOS report on a Strategy for Integrating Satellite and Ground-based Observations of Ozone. WMO GAW Report 140, WMO TD No 1046, 2000.

[RD9] Geo-stationary Satellite Observations for Monitoring Atmospheric Composition and Chemistry Applications, by Jos Lelieveld, Mainz, January 2003. EUMETSAT study for Meteosat Third Generation 2015-2025.

[RD10] Definition of Mission Objectives and Observational Requirements for an Atmospheric Chemistry Explorer Mission, by Brian Kerridge et al. ESA contract 13048/98/NL/GD. Final Report April 2001. ESA SP-1257(4), ISBN 92-9092-628-7, September 2001

[RD11] GeoTROPE, Geo stationary Tropospheric Pollution Explorer, by John P Burrows et al. Proposal in response to ESA 2nd call for Earth Explorer Opportunity Missions. COM2-32, 8 January 2002.

[RD12] TROC, Tropospheric Chemistry and Climate mission by Claude Camy-Peyret et al. Proposal in response to ESA 2nd call for Earth Explorer Opportunity Missions. COM2-35, 8 January 2002.

[RD13] WMO rolling requirement web site

[RD17] PROMOTE, Protocol Monitoring for the GMES Service Element, Atmosphere Service, http://www.gse-promote.org

[RD18] GEMS, Global and regional Earth-system Monitoring using Satellite and in-situ data, EU proposal for an Integrated Project, 30 March 2004.

Chapter Overview

This chapter contains four additional sections. First, in Section 2.2 the method that has been followed to the derivation of geophysical data requirements is outlined. The strategy is shortly summarised, also in comparison to IGACO, and the format of the data requirement tables is shortly explained. Also the definitions of the atmospheric domains that are used in the tables are defined here. In the last two sections of Section 2.2 more general background information is given on the various requirements that are given either in the tables or in the accompanying texts. The requirements that are discussed include coverage, sampling, resolution, revisit time, and uncertainty.

In Section 2.3 the data requirements are defined for the ozone layer theme. In section 2.3.1, 2.3.2 and 2.3.3 the requirements are given for, respectively, protocol monitoring, near-real time data, and understanding. The same format is followed in Sections 2.4 and 2.5 with the data requirements for the Air Quality and Climate theme, respectively.

The Geophysical Data Requirements Tables are listed in the Appendix to this report.

2.2 Derivation of Geophysical Data Requirements

2.2.1 Background

In the CAPACITY user requirements document (also referred to as 'WP1000 report') it is explained that Operational Atmospheric Chemistry Monitoring will contribute to three major environmental themes:

(A) Stratospheric Ozone and Surface UV radiation
(B) Air Quality
(C) Climate

Further, three main drivers have been identified for operational *spaceborne* observations of atmospheric composition. These drivers are

(1) The provision of information on treaty verification and **protocol monitoring**
(2) The facilitation and improvement of operational applications and services, including forecasts, using **near-real time monitoring** information on the atmospheric composition
(3) The contribution to scientific understanding and knowledge acquisition for environmental **assessments** to support policy

Each of the three overall drivers contributes to policy support. The first bullet with direct delivery of required monitoring information, the second with applications and services using actual information and forecasts on the atmospheric state for warning systems and to support real-time decision making, and the third via environmental assessments and their summaries for policy makers (WMO ozone assessments, European and global-scale environmental assessments on Air Quality and IPCC climate assessments).

Furthermore, in addition to the three overall drivers, *spaceborne* operational monitoring of atmospheric composition will be valuable:

- To promote scientific research with unique long-term consistent data products
- To contribute to numerical weather prediction, climate monitoring, and, in broader perspective, Earth system monitoring
- To improve atmospheric correction for surface remote sensing
- To strengthen public awareness on environmental themes

Different levels of information will be needed which can be associated with different user categories. On a first level of information are the users that are involved in the monitoring of protocols and directives (**Compliance User**), e.g. governmental institutes on different administrative levels and international organisations associated with international treaties and protocols. The data requirements of these users are typically level-4 data requirements, such as long-term 3-dimensional global distributions of trace gases, aimed at complete monitoring of the atmospheric state and its evolution in time.

On a second level of information are users that would like to apply the available data products for operational applications and **services**, e.g. meteorological institutes, to improve early-warning systems and to increase public awareness. These users typically need the data in near-real time, i.e., within a few hours after observation. Numerical weather prediction centres may wish to receive level-1 data ('radiances') in order to do processing to level-2 in near-real time and within the running applications.

The services may involve different user categories with specific data requirements, e.g., they may be directed to support policy makers for control strategies and security, health and environmental law enforcement, e.g. on measures to be taken in air pollution episodes. The services can also be directed to the general public for health warnings (concentrations exceeding standards, UV radiation levels) and planning of out-door activities (e.g. a Marathon in Athens) as well as for general awareness. Scientists could use actual information on the atmospheric composition for campaign planning and climate monitoring. Other specific organisations could use the data, e.g. to improve safety of air and road transport by provision of warnings on environmental hazards (forecast of plumes related to volcanic eruptions, extreme forest fires, etc.).

On a third level are scientists assessing the technical basis for abatement strategies, typically summarised in environmental assessment reports (**Technical User**) and the scientists using the information for (fundamental) scientific research (**Research User**). Key to these users is the understanding of the atmospheric state and its evolution. The data requirements are typically enhanced in comparison to the monitoring requirements and these users will require level 1 and/or level 2 data products in addition to level 4. Most important aspect of operational missions for these users is the perspective of unique long-term and homogeneous data sets with global coverage.

Environmental Theme Information	**Ozone Layer & Surface UV radiation**	**Air Quality**	**Climate**
Protocols	UNEP Vienna Convention; Montreal and subs. Protocols CFC emission verification Stratospheric ozone, halogen and surface UV distribution and trend monitoring	UN/ECE CLRTAP; EMEP / Göteborg Protocol; EC directives EAP / CAFE AQ emission verification AQ distribution and trend monitoring	UNFCCC Rio Convention; Kyoto Protocol; Climate policy EU GHG and aerosol emission verification GHG/aerosol distribution and trend monitoring
Services	Stratospheric composition and surface UV forecast NWP assimilation and (re-) analysis	Local Air Quality (BL); Health warnings (BL) Chemical Weather (BL/FT) Aviation routing (UT)	NWP assimilation and (re-) analysis Climate monitoring Climate model validation
Understanding	Long-term global data records WMO Ozone assessments Stratospheric chemistry and transport processes; UV radiative transport processes Halogen source attribution UV health & biological effects	Long-term global, regional, and local data records UNEP, EEA assessments Regional & local boundary layer AQ processes; Tropospheric chemistry and long-range transport processes AQ source attribution AQ Health and safety effects	Long-term global data records IPCC assessments Earth System, climate, rad. forcing processes; UTLS transport-chemistry processes Forcing agents source attribution Socio-economic climate effects

Table 2.1. *Application Areas for Operational Atmospheric Composition Observations*

2.2.2 The Strategy to the Derivation of Geophysical Data Requirements

Reference for our strategy to derive quantitative data requirements from high-level user requirements for CAPACITY has been the compilation of data requirements made for the IGACO theme report. Here the strategy of IGACO is shortly summarised and assessed on its potential usefulness for our derivation of data requirements for future *operational* atmospheric composition measurements.

IGACO

The overall objective of IGACO has been to define a feasible strategy for deploying an Integrated Global Atmospheric Chemistry Observation System (IGACO), by combining ground-based, airborne and satellite observations with suitable data archives and global models. The purpose of the system is to provide representative, reliable and accurate information about the changing atmosphere to those responsible for environmental policy development and to weather and environmental prediction centres. IGACO also aims to improve scientific understanding of the changing atmosphere.

The IGACO system includes the following components:

- Satellite-based instruments preferably mounted on a combination of LEO (low-Earth orbit) polar and GEO (Geo-stationary) equatorial orbiting satellite platforms.
- Networks of ground-based instrumentation to measure surface concentrations, UV radiation and vertical profiles of atmospheric constituents and on a regular basis.
- Regular aircraft measurements of chemical and aerosol species in the entire troposphere, and in the upper-troposphere / lower-stratosphere (UTLS) layer.
- Data assimilation systems capable of integrating the measurements derived from different sources at different times and locations and able to assess the quality and consistency of the measurements.

In IGACO four main atmospheric chemistry themes have been identified:

- Air Quality: the Globalisation of Air Pollution
- Oxidising Efficiency: the Atmosphere as a Waste Processor
- Stratospheric Ozone Shield
- Chemistry-Climate Interaction

For each theme a set of required observables has been established. Unfortunately, within the IGACO process the spatial and temporal resolution, trueness and precision have only been defined for the combination of themes. Also the IGACO data requirements were not necessarily limited to operational observations.

Taking into account financial and logistic constraints a group 1 set of observables has been identified that can be measured by existing or approved observation systems with some limited improvement, mainly in the integration of data. A group 2 set of observables would require development of a next generation of satellites, reinforcement of routine ground and airborne measurement and the development and implementation of a data assimilation system. Both group 1 and group 2 may contain observables that are relevant for future operational systems such as examined in CAPACITY.

CAPACITY

One conclusion to be drawn from IGACO is that for most practical applications satellite measurements are most profitable when these are assimilated into integrated observing systems, such that the satellite measurements are supported by ground-based and airborne observations, and such to create an integrated 4-dimensional view of the state of the atmosphere, using numerical atmospheric (chemistry-transport) models which include the best knowledge of analysed or forecasted meteorological and surface fields.

The integrated approach has also been adopted in CAPACITY, even though this approach is much more complex than the judgement of the potential of satellite observations on their own merits. In the CAPACITY view, the satellite *contribution* to applications should follow from the envisioned role of the operational satellite observations in the integrated observing system. Therefore, data requirements for satelliteborne and ground-based measurements in CAPACITY are based on their envisioned role as first established for each application.

In the user requirements document the relevant themes and user categories for CAPACITY have been identified. These are comparable to the four IGACO themes. Only the IGACO theme on aspects related to changes in the oxidising efficiency, being on its own merely a scientific issue, is in the operational-use oriented CAPACITY structure integrated in the other three environmental themes. For example, the understanding of the 'ozone layer' theme includes the tropospheric changes in UV radiation and composition that are induced by ozone layer changes (and may feedback on it), the 'air quality' theme includes the changes in cleansing of pollutants and the (global) OH budget, and the 'climate change' theme incorporates the OH-related changes in greenhouse gas lifetimes.

In CAPACITY, and this is also different from the IGACO approach, per retrieval product and per atmospheric domain the quantitative data requirements on uncertainty, spatial resolution and revisit time are derived separately for each of the themes and within each theme separately for each of the identified applications.

As said, in order to derive data requirements (typically level-2) based on given user requirements (high level, at best 'level-4') first an assessment needs to be made, per application, on the role that is envisioned for the subsystems, i.e., satellite observations, ground-based observations and auxiliary data sources, respectively, in their contribution to the integrated observing system. The auxiliary data sources include (assimilated) model data as well as geophysical observations other than atmospheric composition (e.g., meteorological variables such as temperature, pressure, cloud properties etc.).

However, even with the roles in the integrated system identified it is very difficult to derive quantitatively for each of the applications what are the specific requirements for each of the subsystems. Extensive assimilation studies would be needed and these studies would be needed for each application separately. For each application a myriad of combinations of different types of satellite and ground-based and in-situ data could be envisioned, each with different assumptions on, e.g., uncertainty and representativeness, and assimilated in different types of chemistry-transport models. Such extensive model simulation sensitivity studies and OSSE's – Observing System Simulation Experiments, using synthetic model-generated measurements to study the impact of a type of observation with specified uncertainty – are outside the scope and resources reserved for the CAPACITY study. On a best-effort basis the currently available expertise with integrated systems making use of present-day data sets, should be exploited. In this respect the CAPACITY study will also draw on the integrated system requirements laid down by IGACO.

The GEMS project, started in 2005, is a project to set up an integrated analysis system along the lines of IGACO. It has four subprojects, namely greenhouse gases, reactive gases, aerosols and (regional) air quality. It will use as many available observations as possible, both satellite and ground-based. The GEMS project will be a demonstration of how possibly newly-developed operational spaceborne measurements could be used in an integrated approach.

Furthermore, although the operational aspect of CAPACITY is quite different from most of the earlier scientific studies on data requirements for atmospheric composition, the specification of data requirements still can build on the heritage of several studies performed in the past. Most relevant in this respect are the ESA proposals for the Earth Explorer mission ACECHEM [RD10], GeoTrope [RD11], TROC [RD12], as well as the ESA study for greenhouse gas emission retrieval from space-based measurements [RD 3]. Requirements on atmospheric composition observations were also established in the EUMETSAT position paper on "Observation requirements for Nowcasting and Very-Short Range Forecasting in 2015-2025" [RD4] and the EUMETSAT study for "Geo-stationary

Satellite Observations for Monitoring Atmospheric Composition and Chemistry Applications in 2015-2025" [RD9].

2.2.3 Data Requirements Table Format and Definition of Height Ranges

The data requirements in this report are tabulated per theme (A,B,C) and per user category (1,2,3) following the structure defined in the user requirements document, i.e., for monitoring / compliance users (A1, B1, C1), for forecast / near-real time applications and services (A2, B2, C2) and for environmental assessments / technical and research users (A3, B3, C3). The requirements are further split into Level 2 satellite data requirements (S), Level 2 ground-based data requirements (G) and auxiliary requirements. Each section starts with some general statements on the envisioned role of satellites, ground-based networks and auxiliary data to the application. Thus, for example, Table A1-S summarises the data requirements from satelliteborne platforms (S) for Theme A (ozone layer), user category 1 (monitoring, compliance user). Table 2.1 summarises the list of data requirement tables. The Data requirements Tables are listed in the Appendix of this report. The auxiliary requirements are described in this chapter.

Table code	Environmental Theme	Application	User category	Subsystem
A1-S	Ozone Layer	Monitoring	Compliance	Satellite
A1-G	Ozone Layer	Monitoring	Compliance	Ground-based
A2-S	Ozone Layer	Forecast	Near-real time	Satellite
A2-G	Ozone Layer	Forecast	Near-real time	Ground-based
A3-S	Ozone Layer	Assessment	Technical/research	Satellite
A3-G	Ozone Layer	Assessment	Technical/research	Ground-based
B1-S	Air Quality	Monitoring	Compliance	Satellite
B1-G	Air Quality	Monitoring	Compliance	Ground-based
B2-S	Air Quality	Forecast	Near-real time	Satellite
B2-G	Air Quality	Forecast	Near-real time	Ground-based
B3-S	Air Quality	Assessment	Technical/research	Satellite
B3-G	Air Quality	Assessment	Technical/research	Ground-based
C1-S	Climate	Monitoring	Compliance	Satellite
C1-G	Climate	Monitoring	Compliance	Ground-based
C2-S	Climate	Forecast	Near-real time	Satellite
C2-G	Climate	Forecast	Near-real time	Ground-based
C3-S	Climate	Assessment	Technical/research	Satellite
C3-G	Climate	Assessment	Technical/research	Ground-based

Table 2.2 *List of the data requirements tables*

Ref code	Environmental Theme					
Requirement / Data Product	Driver	Height Range	Horizontal resolution	Vertical resolution	Revisit Time	Uncertainty

Table 2.3. *Format of the data requirements tables*

The data requirements tables have the general format presented in Table 3. The data products are not sub-divided into mandatory/desired products. In general, it should be understood that typically not the full suite of listed products is mandatory. On the other hand, each of the listed products would contribute with independent information, unless it is explicitly stated that one product is an alternative to another product. We distinguish per data product the relevant height range (for a profile) or a total column, or a partial column (e.g. tropospheric column). In general, the height-range requirements should be interpreted that even when only vertical profile information is required, information from column observations could still contribute to the application, although not fulfilling the vertical resolution requirement. Further the required horizontal and vertical resolution and revisit time are given, for which the first value is a target requirement and separated by a slash (/) the threshold requirement. In the last column the threshold uncertainties that can be allowed for the given (threshold) resolution requirements are presented.

For the height ranges reference is made to the compartments of the atmosphere that are commonly distinguished in atmospheric research. All boundaries should be interpreted as approximate values. In the troposphere distinction is made between the Planetary Boundary Layer (PBL), the Free Troposphere (FT), the Upper Troposphere (UT) and the Tropical Tropopause Layer (TTL). In the stratosphere distinction is made between the lowermost stratosphere (LS), the middle stratosphere (MS), and the upper stratosphere (US). The mesosphere is denoted with (M).

	Tropics	Mid-lat.	Polar
80 km – 35	US+M	US+M	US+M
35 – 20	MS	MS	MS
20 – 16	LS	LS	LS
16 – 12	TTL/UT	LS	LS
12 – 8	UT/FT	UT/FT	LS
8 – 6	UT/FT	UT/FT	UT/FT
6 – 2	FT	FT	FT
2 – 1	PBL	PBL	FT
1 – Surface	PBL	PBL	PBL

Figure 2.1. *The atmospheric compartments that are distinguished for the height-range specifications in the data requirement tables. The boundaries have been set at fixed altitudes and latitudes for simplicity and only represent an approximation to the mean state neglecting atmospheric variability. Tropics [0 – 30 deg], Mid-latitudes [30 – 60 deg], Polar region [30 – 90 deg], in both hemispheres.*

The PBL typically extends up to less than 2 km above the Earth's surface. The PBL is usually thicker above continents than above oceans and typically up to less than 1 km altitude at polar regions. The FT is defined as the region between the top of the PBL and the tropopause. The tropopause in polar regions is typically at an altitude of ~8 km, at mid-latitudes at ~12 km, and at tropical latitudes near ~16 km. The TTL is located in the FT between about 12 and 16 km at tropical latitudes. The UT refers to tropospheric air above about ~6 km altitude. The LS refers to stratospheric air below ~20 km altitude. The MS represents the middle stratosphere between ~20 km (i.e. excluding the lowermost stratosphere) and ~35 km. The upper stratosphere plus mesosphere are defined to extent from ~35 km up to ~80 km altitude globally. No requirements for atmospheric composition above ~80km have been specified. The given domains and their boundaries are all to be considered as a very much simplified of the real, variable atmosphere. Thus, none of the defined boundaries should be interpreted as hard numbers.

2.2.4 Coverage and Sampling Requirements

In general, for each of the listed *satellite products* the target coverage is **global**. This requirement directly reflects the global nature of the three driving environmental themes. Only for the air quality theme, with its additional focus on local, regional and continental scale environmental air quality issues, the required coverage for European-scale operational applications is the European continent, including Turkey, and Europe's surrounding coastal waters as well as the closest parts of the North-Atlantic, which typically impact on the boundary layer in Europe by long-range transport.

For each of the listed *observations from ground-based networks* the target coverage is **global representativeness**, again with threshold coverage for the air quality theme on representativeness for the European continent, including Turkey, Europe's surrounding coastal waters and closest parts of the North-Atlantic. Global representativeness implies that the network is sufficiently spread over the different latitude bands and that each of the stations does not sample exclusively local conditions. In general, it should be realised that the representativeness of any surface-based measurement typically depends on the meteorological conditions. In general, a target and threshold distribution of the ground networks can be established per theme and application.

The general target requirement on sampling is (near-)contiguous sampling. It is clear that no measurement (sub-)system can be envisioned, nor it is desirable or necessary, with continuous and global-scale sampling on the defined spatial resolution and with the defined revisit times. The integration of a single measurement (sub-)system in an integrated system may allow for 'data gaps' in time and space to a certain extent.

On the other hand, in order to have an efficient overall measurement system, the aim of the measurement (sub-)system should be to maximise the number of independent observations to be made by that measurement system, the sampling mostly being limited by the other data requirements on uncertainty, spatial resolution and revisit time. Subsystems with (severe) limitations in coverage and sampling will contribute less to the integrated system and therefore typically should have less priority for operational applications.

2.2.5 Uncertainty, Spatial Resolution and Revisit Time Requirements

The following strategy to the derivation of quantitative data requirements has been followed. At first, for each application a list of observables has been compiled for which the data requirements on spatial resolution and revisit time have been specified. In a next step, and on the basis of the given spatial resolution and revisit times, the requirements for the uncertainty have been specified.

This logic has been followed because the data requirements on spatial resolution and revisit time reflect the atmospheric variability of the observable, which is primarily a function of the time- and spatial scales of the atmospheric and surface processes that are relevant for the observable. Given the relevant temporal and spatial scales the *amount of variability* of the observable on these scales can be investigated. The amount of variability on a certain temporal and spatial scale is relevant for the derivation of the uncertainties. This approach also implies that the different requirements for an observable (uncertainty, spatial resolution, revisit time) cannot be assessed independent from each other.

Uncertainty Requirements

In data assimilation systems it is in the first place the (assumed) uncertainty of the measurement that determines the potential impact of the observation on the system. Therefore, the requirements on uncertainty are the most quantitative and, in fact, leading requirements, at least in comparison to the related requirements on spatial resolution and revisit time. The uncertainty for which the requirement is set will typically contain both a random component (‘root mean square error’) and a systematic (‘bias error’) component. The latter component should be established by a long-term validation with independent measurements. Constant biases are typically not considered most important. Regional biases and random errors are more difficult to define separately, and their relative importance will be dependent on the application (e.g. trends). The relative contributions of random errors and biases will also be very much dependent on the observational technique.

For ground-based observations and in-situ measurements a representation error will contribute to the uncertainty, which should be taken into account in the assessment of the uncertainty requirements for ground-based and in-situ observations. In general, the requirement for these types of observations is that the measurements are sufficiently representative for the given spatial resolution and revisit time. For satellite measurements the representation errors will typically contribute less to the uncertainty, at least as long as the satellite pixel sizes and model grid sizes are of the same order of magnitude or the satellite pixel sizes are larger.

General requirements on sampling and coverage have been specified in Section 2.4. Sampling is also constrained by the given spatial resolution and revisit time requirements. In some cases enhanced temporal or spatial sampling could somewhat relax the uncertainty requirement on an individual retrieval. However, the extent to which relaxation is possible typically depends on the forecast correlation lengths of the assimilation system. These are dependent on atmospheric conditions (see also below). The main limitation on sampling is that the additionally sampled observations need to be independent. A clear advantage of extensive, independent, sampling is that a large number of available observations from prolonged data sets with stable retrievals and limited instrumental drift during the mission lifetime typically will help the data assimilation system to better characterise the random and systematic components of the uncertainty. In this way sampling is related to the uncertainty.

The impact of observations with a certain uncertainty on a data assimilation system will also depend on the (assumed) model forecast uncertainties. These will typically vary from time to time and place to place. This is a complicating factor that has not been taken into account in the derivation of the measurement uncertainty requirements. It can be anticipated that at locations and times with small model uncertainty (e.g. because in-situ observations are available) the uncertainty requirements on the observations can be relaxed to a certain extent. This effect will become more important as models will improve in describing transport and chemistry in the future. On the other hand, atmospheric composition is also to a large extent determined by intermittent processes and ‘unpredictable events’. Because of the unpredictable nature of atmospheric composition (in time and space) it is not desirable to relax a data requirement based on limited model uncertainties in transport or chemistry.

In conclusion, the uncertainties that are given for each of the observables should be read as the maximum (threshold) uncertainty that is allowed in order to obtain information on the observable on the specified spatial resolution and revisit time. Whether the uncertainty is reached with a single retrieval or with a combination of retrievals will depend on the sampling and measurement techniques used. Requirements for these have not been specified.

Horizontal Resolution Requirements

The horizontal resolution requirements are somewhat less quantitative than the uncertainty requirements. As a rule of thumb the horizontal resolution should be at least a factor 2-3 smaller than the error correlation length in the model that is used in the assimilation of the observable. In fact, the assimilation typically combines the available observations within an area defined by the model forecast error correlation length. These are typically a function of altitude in the atmosphere and are mainly determined by the spatial scales of the relevant atmospheric processes and by the resulting spatial variabilities in the observables. Typically, the correlation length decreases from several hundreds of kilometres in the (lower) stratosphere to several tens of kilometres in the lower troposphere and even smaller in the PBL. Correlation lengths in the upper stratosphere and mesosphere are typically smaller than in the lower stratosphere. In some special cases the observation of scales smaller than those defined by the model forecast error correlation length might be very useful as well, e.g., to validate the model on the cascade of processes as a function of spatial scale and parameterisations of sub-grid scale processes.

Vertical Resolution Requirements

The vertical resolution requirements are in the first place related to the gradients of the observable in the vertical direction. Present-day estimates of vertical correlations show very short correlation lengths in the lower stratosphere and UTLS region due to their stratified nature, and much longer correlation lengths in the well-mixed troposphere. In the middle and upper stratosphere the distributions of the observables vary more smoothly in space and the requirements can be limited to a few kilometres in vertical resolution. In contrast, in the UTLS the vertical gradients (and thus the model error correlation lengths) can be very steep and highly variable in time. This results in rather stringent requirements. The vertical gradients in the troposphere typically depend on the synoptic situation and are mainly controlled by convective events and large-scale subsidence. Note that, in contrast to turbulent mixing, convection can either steepen or smooth gradients. The faster overturning in the troposphere transports the information coming from observations more efficiently throughout the model vertical domain than in the UTLS. Therefore the vertical resolution requirements can typically be somewhat more relaxed in the free troposphere than in the UTLS region. Especially in the UTLS region and lower stratosphere the vertical fine-structure of models (dynamics) is not well tested due to a lack of high-resolution vertical information, e.g., with respect to atmospheric waves, and relevant for the general (Brewer-Dobson) circulation.

Revisit Time Requirements

Requirements on the revisit time can, in principle, be determined from examination of the anomaly correlations in an assimilation system. One could argue that if the anomaly correlation drops below a certain predefined threshold, the time evolution as described by the model is not sufficiently adequate and a new analysis based on observations, is needed. The lifetime of the analysis increments depends on the growth of the model forecast error in time. Following this argument the required update frequency would determine the required temporal resolution for an observable. However, it is difficult to estimate the extent to which future (and likely improved) models are able to describe the time evolution of the atmosphere. Current assimilation models have already proven skill for the prediction of stratospheric transport up to more than a week ahead (and possibly longer, depending on the required accuracy). Model skill to describe the evolution of tropospheric transport is much more limited because of the intermittent and unpredictable nature of several processes and event. The model skill on predictability is often limited by the predictability of the meteorological variables (wind, temperature) on which atmospheric composition typically has little influence, at least in the troposphere.

Here, instead of using extensive studies on the anomaly correlation or the model error growth per time step, the requirements on the revisit time for the observables are derived from the typical model forecast error correlation lengths and the atmospheric variability in time of the observable. For example, at the higher altitudes the observables with a diurnal cycle should be observed at least twice daily (e.g. day/night, etc.), while for the other observables daily to weekly observations would probably suffice. The required revisit time typically increases in the lower troposphere and planetary boundary layer, as does the complexity of models to describe the time evolution of the atmosphere. Depending on the relevant atmospheric processes and the geographic location the required revisit time in the PBL can typically vary from several times daily to less than one hour. Finally it is noted that the spatial and temporal resolutions that are or will be used in present-day and future atmospheric models play only a (minor) role for the resolution requirements, because the requirements are determined by the scales of atmospheric processes, which may be either resolved or sub-grid in a model.

2.3 Theme A: Stratospheric Ozone and Surface UV

2.3.1 Protocol Monitoring and Treaty Verification

Relevant Species and Processes

The Montreal Protocol and its subsequent Amendments and Adjustments form the main driver to the monitoring of stratospheric ozone and surface UV radiation. Long-term monitoring is required of the expected decrease in polar and global ozone loss in response to the measures taken based on the Montreal Protocol and its amendments. The ultimate goal is to obtain accurate information on the evolution of the ozone layer (total column) and its effect on surface UV, together with the monitoring of columns of ozone depleting substances (ODS); CFC's and their replacement HCFCs, and halons. Specifically information on the changes (trends) in chlorine loading is needed, both in the troposphere and in the stratosphere.

More detailed policy-relevant information includes the monitoring of the height distribution of ozone and ODS compounds, in addition to total column information. Ozone profile information also allows separation of long-term changes in tropospheric component, mainly relevant to the Air Quality and Climate themes, from changes in the stratospheric component relevant to the Montreal Protocol. These aspects are all considered under 'Assessment' in Section 3.3.

Another user requirement is that the sources of Ozone Depleting Substances (ODS) need to be identified and quantified. Currently this is done from bottom-up country wise official figures. However, independent verification by inverse modelling of the concentration distributions would be highly desirable. Limiting factor for inverse modelling of ODS is however their fairly homogeneous distribution.

The user requirements for operational surface UV radiation monitoring relevant to the Montreal and subsequent protocols need some consideration. In fact the protocols are directed to reduce UV increases that are related to (anthropogenic-induced) changes in total ozone column. On the other hand, the importance of these ozone-related long-term UV changes also need to be viewed in relation to, possibly larger, surface UV changes induced by long-term variations in other processes, including the locally and in time varying effects of clouds, aerosols and surface albedo.

For the long-term monitoring of the surface UV radiation it suffices to monitor on a global scale the *clear-sky UV Index* and the *daily UV dose*. The clear-sky UV Index is an adequate measure that is directly related to (variations or trends in) the total ozone column amount. Next to the total ozone column the main other modulators of the UV Index are the solar spectral irradiance, solar zenith angle and Sun-Earth distance, surface elevation, surface albedo, stratospheric temperatures (via ozone absorption) and aerosol optical parameters. A global daily monitoring of the noontime clear-sky UV Index will also give information on the occurrence of extreme values, which are typically related to ozone depletion events.

The daily UV dose is defined as the 280-400 nm spectrally-integrated erythemally-weighted surface irradiance integrated over daytime. In the interpretation of UV dose variations and trends due to ozone depletion other processes that may result in long-term changes in surface UV radiation levels should be taken into account. Most important for long-term UV dose monitoring, i.e., over decades, are possible systematic changes in the effects of clouds, aerosols, UV surface albedo, and the solar spectral irradiance.

Measurement Strategy and Data Requirements

Given the user requirements on long-term homogeneity and global coverage of the data sets and the trend requirements the most advantageous approach for protocol monitoring is the integration of spaceborne and ground-based data in an assimilation system. In the user requirements document specific requirements have been formulated for satelliteborne total ozone columns (5% rms; 5% bias). The ozone profile should distinguish different atmospheric domains, at least including the lower troposphere, the upper troposphere, the lower stratosphere, and the upper stratosphere and mesosphere. The threshold ozone monitoring requirements can be summarised as follows: Horizontal resolution: 100 km; Vertical resolution: column (mandatory), 4 independent pieces of information (desirable); Temporal resolution 24 hrs; Uncertainty: RMS 5%, bias 5%). Not that some of these requirements are covered under Assessment in Section 2.3.3.

Based on present-day experience with the assimilation of total ozone column information in chemistry-transport models the required information can be obtained by global satelliteborne observations with about 3-days revisit time such as typically provided by ERS-2 GOME. The user requirement on trend detection is rather stringent (~0.1% per year). Although this number applies to the zonal monthly means, the trend requirement is driving the uncertainty requirement of 3% on an individual total ozone column measurement. Neglecting biases, typically ~900 independent measurements per zonal band (of 100 km width) and per month would suffice to reduce uncertainty by a factor 30 as required (3% => 0.1%).

The monitoring of (the trend in) the ODS in troposphere and stratosphere can be performed best using a representative surface network, measuring weekly background surface concentrations and total column amounts of the various regulated ozone depleting substances as listed by, e.g., WMO in the ozone assessment reports. In the data requirement table only the most abundant ODS are listed. Furthermore, especially ODS for which surface-based historical records are available at present are the most relevant for future protocol monitoring. A representative surface network, with at least one background station in each ~10 degrees latitude band, will typically suffice for the determination of total equivalent chlorine in the atmosphere as well as for the derivation of trends in CFC concentrations and trends in their emissions. For the annual trends, typically zonally averaged, weekly representative values with uncertainties of ~2% are needed for the CFCs and other long-lived ODS, and ~5% for the HCFCs.

Independent verification of ODS emissions by inverse modelling of the concentration distributions would be desirable. However, owing to the long chemical lifetime of the ODS, and hence their fairly uniform global distribution this would be a challenging task. On the other hand, it has been shown already that trajectory analyses of surface-based time series of long-lived compounds sufficiently close to emission regions can be used to trace back the emissions to a certain region. Currently it is not foreseen that such detailed studies can be performed on an operational basis. Satelliteborne observations of ODS columns are not likely to contain sufficient information to contribute significantly to inverse modelling of ODS emissions. It is clear that a rather dense surface network would be required to derive country-based (monthly) ODS emission numbers, typically one station per country and further every 10000-100000 km^2.

Operational surface-based observations from a global representative surface network are needed for continuous validation of the ozone column satelliteborne observations. Ozone sonde observations, especially in the polar regions, are needed to provide additional information on ozone that could be difficult to obtain by satelliteborne observations, including the altitude(s) of extreme ozone loss.

The surface UV radiation requirements includes a requirement on long-term time series and regional maps of the daily noontime clear-sky UV Index, typically with at most 1 index point accuracy. It is estimated that the uncertainty requirement to a level-2 UV index product based on satellite observations should be better than ~10% for UV Index higher than 5 index points, and 0.5 index point for smaller UV Index values.

Given the known sensitivity of the UV Index for different parameters the UV Index requirements can be translated into requirements for level-2 products. E.g., maximal a few percent of change in UV Index per change of 0.1 in aerosol optical depth. The relevant products include, next to the total ozone column, the solar spectral UV irradiance and its modulations over time, the aerosol optical depth and absorption optical depth and the UV surface albedo. Trace gases such as NO_2 and SO_2 absorbing in the UV spectral range have a very minor effect on UV radiation levels.

For the surface UV daily dose the estimated uncertainty requirement is 0.5 kJ m^{-2} (for reference: a maximum daily dose at tropical latitudes is ~ 8 kJ m^{-2}, typical values range from 1 to 5 kJ m^{-2}). Apart from the effect of clouds considered below (Section 3.1.3) the same level-2 products as for the clear-sky UV Index are needed to derive the daily UV dose.

Auxilary Data Requirements

The ozone layer monitoring requires assimilation of the observations in an atmospheric model. Therefore, additional information is needed on the meteorological state of the stratosphere. At the time this information is assumed to be adequately available from the analyses of numerical weather prediction models.

For the attribution of UV changes to ozone changes auxiliary information is needed on the global distribution and possible changes over time in:

- 3-D cloud optical and geometric parameters (mainly cloud optical depth and cloud cover)
- Stratospheric temperatures (determining the UV absorption for a given ozone amount)
- The UV extraterrestrial solar spectrum, covering the 200-400 nm spectral range
- 3-D aerosol optical parameters in the UV (mainly aerosol optical depth and single scattering albedo)
- 2-D UV surface albedo global distribution

The latter three bullets are covered in the data requirement table of A1-S. Stratospheric temperatures are assumed to be adequately available from the analyses of numerical weather prediction models.

Setting data requirements for detailed cloud information is outside the scope of the CAPACITY study. However, given the large, often dominating effect of clouds on the daily UV dose and its changes over time and place, the required cloud information needs to be quite detailed in time and space in order to be able to derive information on surface UV variations and trends that can be related to ozone changes as required here for protocol monitoring. Typically, for the interpretation of the UV dose accurate cloud information is needed on cloud cover and cloud optical depth as a function of time over the day with time steps of about an hour or less. Here, it is assumed that the required information on cloud parameters will be adequately available from existing or planned meteorological platforms (e.g. MSG, GOES). A good cloud mask (on/off) is the most crucial requirement.

In the mapping of the UV daily dose the various level-2 data products that are needed are typically gridded (level 3-4) before these are combined. Requirement on co-location of the various products are therefore not considered very stringent. The different products may be derived from different platforms, including for example a platform in low orbit for total ozone, the solar spectrum, aerosols, and surface albedo, and a geostationary platform for variables that typically change significantly over the day (cloud parameters and, possibly, aerosol parameters).

2.3.2 Near-Real Time Data Requirements

Relevant Species and Processes

Forecasts of ozone fields and surface UV radiation are required for different user groups. Near-real time ozone data are required for improved radiances in Numerical Weather Prediction models and as input data for surface UV forecast. For forecasts a data assimilation system is needed to integrate the near-real time observations and to combine these with transport information from the model forecast. It has been shown that with present-day numerical weather prediction models reliable total ozone and clear-sky UV Index forecasts are possible up to ~1 week ahead.

Near-real time information on the ozone layer is also required during periods of severe (polar) ozone loss to inform policy makers, the media and the general public. Currently, near-real time data relevant to Arctic ozone loss has been intended for scientific use only, e.g., related to Arctic measurement campaigns. Especially extensive ozone loss that takes place in the Arctic during cold winters is a cause of great concern due to its proximity to inhabited areas. Forecast of, e.g., the Antarctic vortex break-up would contain important information especially for some countries in the Southern Hemisphere including Argentina, Chile, New Zealand and some small islands.

For surface UV radiation forecasts, such as provided in most countries by the meteorological institutes, total ozone column forecast information is needed, typically for a few days ahead. Additional forecast information is required on clouds, aerosols and surface albedo. However, given the present-day uncertainties that are associated with the forecast of these additional parameters, current forecasts of surface UV radiation are often limited to so-called clear-sky values (at most including a fixed aerosol correction and in some countries taking into account known surface albedo variations). The reported clear-sky therefore typically represent the most extreme case. Near-real time observations of aerosols and surface albedo are needed to reduce the uncertainty in their effect on the clear-sky UV predictions.

In some countries, an uncertainty range is presented on the UV Index forecast where the given range mainly reflects the prediction of the possible reduction of UV radiation by clouds. Improved cloud forecasts (mainly on cloud cover and cloud optical depth) would help to reduce the uncertainties that are associated with cloud predictions.

Note that UV Index forecasts need to report the highest expected value for the day, which is typically around noontime.

Measurement Strategy and Data Requirements

Modelling of the evolution of the ozone layer over a couple of days (e.g., up to ~10 days) requires information on the full three-dimensional ozone layer distribution. Based on the initial field the meteorological forecasts will be used to transport ozone in all dimensions and this will result in a new ozone field from which the required forecast of the spatial distribution of the ozone columns can be derived.

In order to accurately forecast ozone columns, near-real time satelliteborne ozone profile measurements are needed in the UTLS region and above. In the troposphere a measurement of the tropospheric column suffices. Total ozone column observations can also be used, although at the expensive of accuracy. Typically for the ozone profile the required vertical resolution decreases from about 2 km (threshold) in the UTLS region to ~5 km in the upper stratosphere and mesosphere. If the complete ozone profile cannot be covered by the measurements, additional information will be needed from measurements of the total ozone column.

Near-real time availability of surface-based observations of total ozone columns is needed to complement and validate the satelliteborne observations. Furthermore, a representative ozone sonde network is needed for validation of the assimilated ozone distribution. In-situ ozone profiles are also needed to enhance the vertical profile information in the troposphere and lower stratosphere.

Both ground-based measurements and spaceborne estimates of the UV dose and UV Index are needed for the validation of the UV forecasts. Although the quality of (derived) surface UV radiation measurements is highly correlated with the quality of the total ozone observations, some differences between both data sets will occur because clear-sky surface UV radiation products are additionally weighted with solar zenith angle, aerosol load, and surface albedo. Some information on possible long-term changes in the incoming UV solar irradiance at the top of the atmosphere would also contain valuable information for UV forecasts.

A complicating factor for validation of the satelliteborne surface UV estimates is the variable presence of aerosols and clouds. Near-real time observations of the UV spectral aerosol (absorption) optical depth and UV spectral surface albedo will help to reduce uncertainties in UV forecasts. The required spectral range for these products is the 280 – 400 nm spectral region. The required spectral resolution is typically 5 to 10 nm in the UV-B range (280 – 320 nm) and 10 to 20 nm in the UV-A range (320 – 400 nm).

A requirement for the forecast model is that the dynamics of the stratosphere are well-predicted and also that changes in ozone due to dynamics can be distinguished from changes in ozone that are related to chemical and/or radiative processes. Good vertical resolution is crucial to better represent stratospheric waves. It has been shown that inclusion of a parameterisation of heterogeneous ozone loss processes can improve the forecasted ozone distribution. For the stratospheric radiation budget the most important gases to assimilate together with ozone are H_2O, CO_2, CH_4, and N_2O.

Assimilation of tracer observations of SF_6 or CO_2 could be used to better separate between ozone transport and ozone chemical processing. Currently, parameterisations on ozone loss are based on the prediction of temperature. Ozone loss processing can be better constrained by observations of PSCs, enhanced ClO, and aerosol extinction.

Operational in-situ aircraft measurements in the UTLS region, co-located with ozone observations, of H_2O, CO, HNO_3 and HCl would be desirable to better constrain the stratosphere-troposphere exchange processes. Operational spaceborne observations of these gases in the UTLS region could possibly contribute as well.

Finally, near real time data delivery for this application implies that the data needs to be available to an operational modelling environment within a couple of hours after observation. In that case a significant part of today's observations can still be used for the analysis on which the required forecast for tomorrow (etc.) will be based.

Auxilary Data Requirements

Ozone forecasts rely on an operational assimilation system including the meteorological analysis and forecast of stratospheric transport. The required meteorological fields, up to at least one week ahead, can only be delivered by numerical weather prediction centres. Therefore, it is foreseen that forecast services will be run by these meteorological centres. The operational atmospheric composition products will contribute to the overall assimilation system. Significant experience will be obtained in the GEMS project that will start in 2005.

UV radiation forecasts are typically most relevant for clear-sky conditions as these typically represent the maximum level that can possibly be obtained. However, forecasts including the effect of clouds would be more realistic. Therefore, improved all-sky UV radiation forecasts would profit from improved forecasts of cloud parameters. Most important parameters for all-sky UV Index forecasts are, next to the information on ozone, aerosols and surface albedo, cloud cover, especially around noontime, and cloud optical depth.

For forecasts of the UV dose, a forecast of (the distribution of) the sunshine duration over the coming days would be the most crucial parameter, together with the above-mentioned cloud parameters relevant for the UV Index.

Improving cloud forecasts, especially with the aim to improve surface radiation forecasts is extremely challenging. Even with near-real time availability of cloud observations current scientific knowledge of cloud processing likely does not allow accurate forecasts of cloud distribution for the purpose of improving UV forecasts for typically 24 hours ahead. No requirements on cloud parameters have been formulated in CAPACITY.

Global radiation (pyranometer) measurements from the surface radiation networks could be another independent set of observations that can account for the cloud and aerosol effects on UV. Also, forecasts of global radiation are becoming available from numerical weather prediction centres and these could give additional information that is useful to improve upon the UV forecasts.

2.3.3 Assessment

Relevant Species and Processes

More detailed policy information than required for direct protocol monitoring (total ozone column, surface UV; Section 3.1) will be based on the monitoring of the height distribution of ozone and ODS compounds, related compounds and parameters other than ozone that affect the surface UV radiation. For example, ozone profile information is necessary in order to separate long-term changes in the troposphere ozone component, mainly relevant to the Air Quality and Climate themes, from changes in the stratospheric component relevant to the Montreal Protocol.

For the ODS altitude information would also give indication on the effectiveness of treaty implementation. Desirable is the stratospheric halogen loading, which includes also reservoir species such as HCl, $ClONO_2$, HBr and $BrONO_2$. In addition, monitoring of these reservoir species might be relevant for another reason: it is anticipated that changes in reservoir species typically would precede changes in total chlorine content and therefore would give an early indication of changes in equivalent chlorine. Certain active chlorine and bromine components (ClO and BrO) and PSCs are indicators of the amount, severity and extent of ozone depletion events, which is additional relevant information for treaty verification.

The main drivers for a better understanding of the ozone layer evolution and long-term changes in surface UV radiation are the following long-term science questions:

- Understanding of the trends in total ozone, largely by examination of the evolution of the ozone layer and the changes in the ozone distribution over time
- Understanding of the effects on the ozone layer of the policy measures taken in response to the Montreal Protocol and its different amendments
- Understanding of the global ozone chemical budget, including the relative roles of denitrification, heterogeneous chemistry and other ozone loss processes
- Understanding of the processes resulting in interactions between ozone recovery and climate change, related to radiation, dynamics and/or chemistry

- Understanding of the long-term changes in surface UV radiation levels, their attribution to either total ozone changes or other processes, and their effects on health and the environment
- Understanding of the distribution of the ozone depleting substances and the trends in their concentrations

To answer these questions scientific users require long-term global monitoring of the three-dimensional distribution of ozone, ozone depleting source gases, and some other long-lived key gases in the stratosphere, as well as stratospheric aerosols and PSCs. For understanding changes in surface UV radiation additional information is needed on the various processes that affect surface UV radiation, most importantly next to ozone, clouds, aerosols, surface albedo and the solar spectrum.

Long-term operational data sets will be most essential to validate 'slow' processes in atmospheric chemistry models. With 'slow' processes reference is made to processes that are predicted to have significant effect on, e.g., the ozone layer on the long term although the direct effect can difficult to obtain from dedicated measurements that are typically limited to short time periods. One such 'slow' process is, e.g., the continuous increase of CO_2 and other greenhouse gases concentrations in the atmosphere, that is predicted to affect the ozone layer by inducing changes in, e.g., the temperature distribution in the stratosphere. Another example is the observed slow increase in stratospheric water vapour, partly caused by CH_4 increases, but largely not well understood. Further, the increase in stratospheric N_2O concentrations is expected to enhance the relative role of the nitrogen cycle in stratospheric chemistry.

Operational measurements of atmospheric composition can mostly be limited to the longer-lived compounds. The measurement of short-lived compounds on an operational basis is considered of less relevance because a lack of scientific understanding of a certain chemical or physical process is likely to benefit more from dedicated (campaign) measurements than from operational data. Operational measurements, however, can help to quantify the relative importance of different (fast) processes on the long term, e.g. in relation to the contribution of the hydrogen, nitrogen and halogen cycles to the chemical ozone budget.

Measurement Strategy and Data Requirements

Crucial for understanding of the long-term evolution of the ozone layer is the monitoring of changes in the vertically resolved concentration distributions in the global stratosphere. Long-term ozone changes occur at different altitudes and at each altitude different chemical, dynamical and radiative processes play a role. Vertical resolution is most critical in the UTLS region where stratosphere-troposphere exchange processes result in large gradients in the ozone distribution. A target vertical resolution of 1 km is given for spaceborne ozone observations, with a threshold of 3 km resolution. Especially in the latter case the spaceborne observations in the UTLS would benefit if complemented by more detailed ground-based and airborne observations. In the middle and upper stratosphere the ozone distribution is less variable and the required vertical resolution is typically relaxed to 3-5 km. Total column information is needed in cases that the vertical profile is not covered in all atmospheric domains. Spaceborne observations of the tropospheric column (in combination with an averaging kernel) would help to distinguish from total ozone observations between changes in tropospheric ozone and changes in stratospheric ozone. Ground-based networks and airborne UTLS observations are needed to enhance the profile information on tropospheric ozone and to better quantify changes in the net ozone flux from the stratosphere into the troposphere.

Monitoring of the total stratospheric halogen loading requires satelliteborne stratospheric profile observations of the main reservoir gases: HCl, $ClONO_2$, HBr and $BrONO_2$. The reservoir gases are spatially and temporally much more variable than the ODS. Vertical profiles with about 3 km resolution covering the lower and middle stratosphere suffice. Additional HNO_3 stratospheric profile information is desirable to observe possible long-term changes in denitrification. Typically a zonal mean uncertainty of ~20% could be allowed for data that is representative for a few days to one week.

For some gases an uncertainty for a 1000km-average has been specified to account for anticipated longitudinal variations in these compounds.

The uncertainty requirements for ClO (for enhanced levels) and BrO of ~50% are set, e.g. as occurring in spring in the polar stratosphere. For protocol monitoring these short-lived gases, responsible for at least 50% of springtime stratospheric ozone loss, are mainly desirable to detect the number, location and extent of events with excessive ozone loss, i.e. statistics. For the same reason the data requirement on PSCs is also limited to detection only (instead of full characterisation, see the section on ‘ozone layer: understanding’).

Several long-lived gases are important to be monitored for a better understanding of the evolution of the ozone layer. These include at least H_2O, CH_4, N_2O and HNO_3. The gases play multiple roles in the stratospheric physical system. Most important is the long-term trend of these gases as well as information on possible changes in their vertical and zonal distributions. E.g., changes in the HNO_3 distribution can be related to long-term changes in denitrification. Also NO_2 observations are considered very useful in this respect.

Ground-based networks of surface concentrations and total columns are most suited for determination of trends in ozone depleting substances (ODS), of which the most important are CFC-11, CFC-12 and HCFC-22. Desirable for understanding the ozone layer evolution in response to policy measures taken in response to the Montreal Protocol and its amendments would be further the measurement of the gases CFC-113, HCFC-123, HCFC-141b, HCFC-142b, CCl_4, Halon 121, Halon 1301 and Halon 2402. In this list CH_3CCl_3 is neglected because it is assumed to be of minor relevance for ozone depletion after 2010. Satelliteborne observations are useful to complement the ground-based measurements and to verify the representativeness of the ground-based networks for global trend determination of the ODS concentrations. Satelliteborne profile observations of other source gases such as CH_3Cl and CH_3Br as well as reservoir gases such as HCl, $ClONO_2$ would further aid to understanding of the diminishing role of the anthropogenic ODS to the ozone layer evolution.

Satelliteborne measurements of SO_2 and volcanic aerosol would be needed for understanding the ozone layer evolution in case of severe volcanic eruptions polluting the stratosphere for a couple of years, e.g., comparable to effect of the Pinatubo eruption in 1991.

Understanding of surface UV radiation changes and their possible effects on health and the environment requires long-term satelliteborne monitoring of the 3-D ozone distribution (i.e., preferably ozone profiles), the UV aerosol optical depth, the UV aerosol absorption optical depth or single scattering albedo, the UV surface albedo, and the extraterrestrial solar spectrum in the UV range.

Finally, operational ground-based measurements from a representative global network are needed for continuous validation of the mentioned satelliteborne measurements and derived surface UV products.

Auxilary Data Requirements

For the ozone assessment the interpretation of the combination of ground-based observations and satelliteborne observations would be most beneficial if the observations are assimilated in chemistry-transport models. The main auxiliary requirement is therefore on the availability of state-of-the-art chemistry-transport models, preferably covering the atmosphere from the surface to the mesosphere and making use of analysis fields of numerical weather prediction models, detailed emission databases (both natural and anthropogenic), and adequate chemical schemes.

In addition, the interpretation of long-term variations and trends in stratospheric composition requires information on climate and climate evolution. Especially relevant is climate monitoring of the variations and trends in the main meteorological parameters in the stratosphere and mesosphere (temperature, air density, winds, Brewer-Dobson circulation, etc).

2.4 Theme B: Air Quality

2.4.1 Protocol Monitoring and Treaty Verification

Relevant Species and Processes

Within the Air Quality theme the main drivers for protocol monitoring are the EMEP and Gothenburg Protocols of the UN/ECE CLRTAP convention, the National Emission Ceilings, as well as complementary regulations related to EU Air Quality policy, e.g. in relation to the CAFÉ (Clean Air for Europe) program (Table 1). The user requirements include the monitoring of the total abundances and concentration distribution of the regulated gases and aerosols as well as the detection and source attribution of the related emissions for verification. In order to observe peak concentration levels, e.g. as related to rush hours or to accidental chemical releases, typically monitoring of hourly surface concentrations are needed. In order to monitor the effect of policy measures it is needed to be able to derive information on trends in concentrations and emissions within a time frame of maximum a few years.

Air Quality data requirements primarily should respond to the need for information on pollution levels at ground level and in the planetary boundary layer (PBL, typically between surface and ~1-2 km altitude) where they impact on the health and safety of people and of the biosphere. However, additional information on the composition of the adjacent free troposphere is also important as boundary condition to the PBL. The long-range transport and free-tropospheric photochemistry determine the background concentrations of the longer-lived pollutants on which locally pollution builds up.

The compounds for which the surface concentrations are regulated include O_3, SO_2, NO_x, Particulate Matter (PM10, PM2.5, PM1 in ($\mu g\ .m^{-3}$), denoting particles with diameters smaller than, respectively, 10, 2.5 and 1 microns), CO, benzene (C_6H_6), Poly Aromatic Hydrocarbons (PAHs), and some heavy metals (Pb, Ni, As, Cd, and Hg). Regulations on PM1 are anticipated.

Driving the requirements on emissions are the National Emission Ceiling Directives for SO_2, NO_x, Volatile Organic Compounds (VOCs), NH_3 and fine particulate matter. Also the CLRTAP convention, which includes Europe, Russia, US and Canada, sets emission ceilings on SO_2, NO_x, VOCs and NH_3, by the EMEP and Gothenburg protocols. The Gothenburg protocol also regulates surface ozone levels.

In reference to the GMES-GATO [RD2] it has been recommended in the user requirements document to anticipate on possible future regulation of ship emissions. The most important ship emissions include CO, NO_2, SO_2 and particles. Concentrations of these compounds need to be monitored from operationally shipping in harbours, main waterways, and over coastal waters.

Measurement Strategy and Data Requirements

Traditionally, the requirements for monitoring and verification of air quality have been formulated based on the means already available for verification and enforcement, which consist of ground-based networks at the local and regional authority level. Even though the data quality issue is addressed in the EC framework directive, at present these data are often of limited use in a global observation network, through lack of standardisation of instruments employed and data generated. Furthermore, continental and hemispherical or global coverage can practically not be obtained by ground-based networks. An optimal strategy for air quality protocol monitoring and verification would be based on a synthesis of satellite observations, ground-based networks and air quality model information through data assimilation on different spatial scales.

It has been shown that local to regional air quality models are very useful to complement the ground-based networks, e.g. to interpolate in time and space. However the models are also essential because these include meteorological information on the boundary layer, e.g. based on numerical weather prediction model output. For example, the boundary layer height is crucial for the surface concentration levels that are attained as it determines the extent of the planetary boundary layer and as such the atmospheric volume in which surface emissions are injected. Other meteorological variables that can be delivered by the air quality model and that are essential for the surface pollution levels include the wind speed and direction, turbulent mixing, temperature, water vapor, UV radiation, clouds and convection. In addition the model can include detailed information on natural emissions, also based on surface characteristics such as vegetation and snow cover. For example, ozone levels in rural, moderately polluted regions are known to be very sensitive to meteorology-dependent isoprene and monoterpene emissions.

Satelliteborne observations can help to fill in gaps in the surface networks, although global-scale satellite measurements cannot be expected to be of sufficient resolution and accuracy to deliver accurate information on local surface concentration levels. Satelliteborne observations are crucial, however, for the boundary conditions of the air quality models. These models are typically limited to a certain region and therefore highly dependent on appropriate boundary conditions, especially for the meteorology and the longer-lived compounds. These boundary conditions, e.g. for chemical compounds over the oceans, can typically be delivered by global model output in which satellite observations of tropospheric composition have been assimilated.

Inverse modelling will be needed to derive emissions based on concentration distributions. Currently, the intrinsic limitations of ground-based observations also hamper the emission verification using inverse modelling. Independent observations from satellites will help to better constrain the inverse modelling. Note that especially the performance of the air quality model will be crucial for the quality of the emissions that can be inferred using inverse modelling techniques. It is anticipated that with the increasing level of detail incorporated in the air quality models the uncertainties related to inverse modelling of emissions will become smaller in the coming years. In order to derive emissions on a country-by-country basis or better the density of the surface network should be typically 10000-100000 km^2, with at least one measurement station per country.

The surface network for protocol monitoring should be representative for the polluted regions in Europe and include at least surface concentration measurements of O_3, SO_2, NO_x, PM10, PM2.5, PM1, CO, benzene (C_6H_6), Poly Aromatic Hydrocarbons (PAHs), ammonia (NH_3) and heavy metals (Pb, Ni, As, Cd, and Hg). Note that in CAPACITY requirements for ground-based measurements are limited to compounds for which satelliteborne observations play a role, i.e., requirements for, e.g., PAHs, ammonia and heavy metals have not been derived. Long-term homogeneous measurement series are needed in order to derive trends in the surface pollution levels. About 10% uncertainty on individual measurements should be sufficient both for the hourly peak levels and for the detection of small long-term trends in monthly mean peak values.

The satellite measurements of trace gases should include preferably tropospheric profiles of O_3, SO_2, NO_2, CO and formaldehyde (CH_2O), at least separating the boundary layer from the free troposphere. The threshold vertical resolution requirement is a tropospheric column, in combination with an averaging kernel in order to have information on the sensitivity of the satellite measurement as a function of altitude. Note that formaldehyde is required because it will contain important information to constrain the VOC emissions.

The required revisit times are typically between half-hour (target) to several hours and are directly related to the protocol requirements to observe hourly peak pollution values, in combination with the fast chemistry and mixing time scales of the planetary boundary layer. The revisit time requirements are typically for daytime only (this is the threshold requirement) as photochemistry is a major driver for the pollution levels. The extension to full 24h coverage, i.e., including the night-time evolution is a target requirement and can be a useful additional constraint to air quality models, especially for ozone and nitrogen compounds (NO_X, N_2O_5, HNO_3, PAN).

The uncertainty requirements typically do not pertain to very clean or background levels. However, it is still needed to measure in the background atmosphere and to assign these pixels as being background or below the detection limit. This is especially true for SO_2, NO_2 and CH_2O satellite observations for which the threshold uncertainty is expressed in absolute terms. Column amounts of $<1.3 \cdot 10^{15}$ molecules cm^{-2} correspond to background conditions, with column average concentrations below 1 ppbv. The uncertainty is given in absolute terms ($1.3 \cdot 10^{15}$ molecules cm^{-2}) and corresponds, e.g., for NO_2 with 100% relative uncertainty for a column of $1.3 \cdot 10^{15}$ molecules cm^{-2} to <10% uncertainty for columns larger than $1.3 \cdot 10^{16}$ molecules cm^{-2}. Note that satellite NO_2 measurements are assumed to suffice for constraining NO_x emissions and NO_x ambient levels. This assumption sets some basic requirements on the chemical scheme that is to be used in the Air Quality model for the NO/NO_2 conversions.

Maximum uncertainties for PM10 and PM2.5 surface concentrations have been fixed in absolute terms at two times the measured background concentration in Europe (van Dingenen et al., Atmos Environ., 38, 2561-2577, 2004). For PM1 requirements could not be specified as information on the background concentrations is lacking.

The vertical resolution requirements on the satellite observations of aerosol optical depth are similar to the satellite requirements on trace gases, with a target to distinguish between aerosols in the boundary layer and free troposphere and a threshold for the tropospheric aerosol optical depth. The required uncertainty (0.05) is again expressed in absolute terms and based on different earlier assessments. The aerosol optical depth observations can be used to constrain the surface concentrations of PM. Information from satellite on aerosol type would be desirable.

The requirement on ship emissions extends the need for surface measurements to coastal waters. These ground-based measurements should include at least CO, NO_2, SO_2 and particles. The same compounds over coastal waters measured from satellite would add significantly to the ship data.

In addition to the monitoring network for surface concentrations, ground-based observations are also needed for the validation of the models and satellite observations in the troposphere. The observations should include ozone profiles from the sonde network as well as tropospheric column data at representative sites for the validation of the modelled and satelliteborne observations of tropospheric ozone. Lidar observations at specific sites are very useful to validate the vertical tropospheric profiles of O_3, NO_2, SO_2 and CH_2O. Boundary layer concentration profiles from towers at a few locations would also help to validate satellite data and models.

Auxilary Data Requirements

Air quality protocol monitoring heavily relies on the combination of ground-based observations, air quality models and satellite data. The main auxiliary requirement is therefore on the availability of state-of-the-art air quality models making use of analysis fields of numerical weather prediction models, detailed emission databases (both natural and anthropogenic), adequate chemical schemes and detailed descriptions of surface-atmosphere exchange processes.

2.4.2 Near-Real Time Data Requirements

Relevant Species and Processes

The main societal drivers for air quality forecasting are health and safety warnings (Table 1). Surface concentration predictions are needed from local street-level to regional and national scales. Typically the maximum delay time allowed for data delivery is very short, about 30 minutes. The so-called Air Quality index, according to EC directives, is based on a mixture of O_3, NO_2, PM10, SO_2, and CO. These compounds are affecting respiratory health. Because particle size is likely important, distinction is made between PM10, PM2.5 and PM1. Particles are possibly also related to cardiovascular health (Chapter 1). Metals in particles could also be an issue.

With respect to safety natural hazards such as volcanic eruption, forest fires and man-made hazards such as biomass burning and chemical and nuclear releases require plume transport and dispersion model forecast fed by observations. An additional driver here is air traffic management, including both air routing and early warnings for forementioned unpredictable events.

An important requirement for health and safety is further near-real time source detection and attribution of the emissions of aerosols and aerosol and ozone precursors (NO_2, SO_2, and CO).

Additional information on methane (CH_4), water vapour (H_2O), formaldehyde (CH_2O) as well as the UV-VIS photolysis rates is important for the forecasting of the photochemical activity. These observations are needed to constrain the chemical conversion rates and help to determine the atmospheric residence time of pollutants.

Measurement Strategy and Data Requirements

The optimal strategy for air quality forecasting is similar to the strategy for air quality monitoring described in section 2.4.1 and based on a synthesis of satellite observations, ground-based networks and air quality model information through data assimilation on different spatial scales. The main difference is the requirement on the timely availability of the forecast information.

Typically, environmental agencies require air quality forecasts for the day to be available in the early morning. The time delivery requirement on the observations for air quality forecasts is therefore mainly determined by the need for the data to be available for the integrated forecast system at the time that the analysis run is performed on which the forecast run will be based. In practice, the analysis run will have to be performed in the late evening or early night in order to do a forecast run that finishes in early morning. The minimum delivery time requirement is therefore about several hours. Given that the daytime observations are most relevant, the most stringent delivery requirements are for the last daytime measurements of the day. The user requirements on the timely availability of the forecasts prevents the need for observations of the same day as for which the forecast is being made. This is true for satellite observations as well as for observations of the ground-based networks.

The revisit time satellite data requirements are for daytime only (threshold), except for N_2O_5, HNO_3 and PAN for which especially nighttime observations would be desirable, given their role in the nighttime NO_y budget, which is an important constraint on the amount of NO_x released from reservoir species after sunrise. The threshold revisit time requirements of 2 hours are mainly related to the diurnal cycle of air pollution levels as well as the short timescales of the mixing and chemical processes in the planetary boundary layer.

The satellite measurements of trace gases should include preferably tropospheric profiles of O_3, H_2O, SO_2, NO_2, CO and formaldehyde (CH_2O), at least separating the boundary layer from the free troposphere. The threshold vertical resolution requirement is a tropospheric column, in combination with an averaging kernel in order to have information on the sensitivity of the satellite measurement as a function of altitude. Note that formaldehyde is required because it contains information on the amount of photochemical activity caused by hydrocarbons. Water vapour profile information is important for the effect of relative humidity on aerosols as well as for the primary OH production, which controls the photochemical activity together with the ozone concentration and UV-VIS actinic flux.

The aerosol requirements on the satellite observations are on the aerosol optical depth and the aerosol type, with a target to distinguish between aerosols in the boundary layer and free troposphere and a threshold for the total tropospheric aerosol optical depth. The required uncertainty (0.05) is expressed in absolute terms and based on different earlier assessments. The aerosol types to distinguish include at least standard categories such as sulphate, dust, sea salt, organic carbon (OC), black carbon (BC), and mixed aerosol. The requirement on aerosol type is that misassignments should be limited to less than about 10% of the cases.

For air traffic management the threshold coverage requirements on aerosol optical depth and SO_2 are global scale, while all other air quality forecast applications have a threshold coverage requirement which is limited to Europe and its coastal waters (see Section 2.4)

Ground-based networks can significantly add to the air quality forecasts, especially by adding information on the local scale. The measurements should preferably include O_3, and H_2O profiles from sonde measurements, as well as surface concentrations of O_3, SO_2, NO_2, CO, CH_4 and CH_2O from a representative network. Information on surface CH_4 concentrations is relevant, because CH_4, although being relatively well-mixed, is an important competitor for the OH radical, and therefore variations in its abundance affects the lifetime of other compounds, especially CO.

Finally, near real time data delivery for this application implies that the data needs to be available to an operational modelling environment within a couple of hours after observation. In that case a significant part of today's observations can still be used for the analysis on which the required forecast for tomorrow (etc.) will be based. It should be noted that current practice of data time handling at ECMWF is not favourable for Air Quality forecasts. Data are collected twice a day (till 3 am and 3 pm) to provide forecasts in the morning and evening. For Air Quality forecasts it would likely make sense to include also the late afternoon observations of today in the Air Quality forecast for tomorrow, which should be available to operational agencies in the very early morning of the day to come.

Auxilary Data Requirements

Air quality forecasting heavily relies on the combination of ground-based observations, air quality models and satellite data. The main auxiliary requirement is therefore on the availability of state-of-the-art air quality forecast model making use of analysis fields of numerical weather prediction models, detailed emission databases (both natural and anthropogenic), adequate chemical schemes and detailed descriptions of surface-atmosphere exchange processes.

2.4.3 Assessment

Relevant Species and Processes

In order to feed into environmental assessments and within the Air Quality theme the main drivers for understanding are the following long-term science questions:

- What is the impact on air quality of the spatial and temporal variations and possible trends in the **oxidising capacity**?
- What is the impact on air quality of spatial and temporal variations and possible trends in the **long-range transport** of longer-lived compounds and aerosols?

- What is the impact on air quality of long-term changes in the distribution and total burden of the tropospheric ozone, carbon monoxide and methane **background levels**?
- Can we relate the observed changes in atmospheric pollution levels to changes in certain emissions (**source attribution**)?

To answer these questions scientific users require long-term data sets of the total abundances and global concentration distribution of the pollutants as well as the detection and source attribution of the related emissions. For trend detection typically, monthly mean to annual values are needed in order to be able to relate changes in concentration levels to changes in emissions, possibly in response to policy measures.

The oxidising capacity of the atmosphere is largely governed by the OH and tropospheric ozone budget. Analysis of the causes for changes in the OH production and loss rates can be derived from simultaneous measurements of the global distribution (and spatial and temporal changes therein) of the longer-lived compounds in the OH budget, including H_2O, O_3, NO_x, CO, CH_4, CH_2O and higher hydrocarbons, in combination with numerical modelling of chemistry, transport and mixing, emission and deposition, and UV-VIS radiative transfer for the photolysis rates.

Important for the tropospheric ozone budget are the mixing and transport processes including stratosphere-troposphere exchange, ozone deposition, the ozone precursor gases (mainly NO_x, CO and CH_2O) and their chemistry, photolysis rates (mainly of NO_2 and O_3), water vapour and temperature. *The trend of tropospheric ozone* requires accurate monitoring of the tropospheric ozone profile.

Information on long-range transport is most important for CO, NO_x, NO_y, O_3, and aerosols.

The trend of tropospheric ozone, carbon monoxide and methane requires accurate monitoring of the tropospheric ozone profiles and CO and methane surface concentrations at background stations.

Inverse modelling will be used to derive emissions. Required emissions include aerosol emissions and aerosol and ozone precursor emissions including SO_2, NO_2 and CO.

Measurement Strategy and Data Requirements

The target coverage for understanding air quality issues should be global. The threshold coverage for the planetary boundary layer can be Europe, incl. coastal waters, and for the free troposphere the threshold coverage includes at least parts of the North-Atlantic which impact on the surface air quality levels in Europe. The European scale mainly refers to use in scientific assessments by, e.g., the European Environmental Agency and understanding of European scale air quality issues.

For understanding of the oxidising capacity of the atmosphere related to air quality issues measurements are needed of the global distribution (and spatial and temporal changes therein) of the longer-lived compounds in the OH and tropospheric ozone budgets, including H_2O, O_3, NO_x, CO, CH_4, CH_2O and higher hydrocarbons, most notably isoprene and monoterpenes. Additional information would come from observations of the UV-VIS actinic flux, and N-reservoir species, especially at night, including HNO_3, PAN, organic nitrates and N_2O_5.

The revisit time satellite data requirements are typically for daytime only. However, for example for O3, CO, and especially N_2O_5, HNO_3 and PAN nighttime observations would certainly be worthwhile. The N-compounds would give information on the nighttime NO_y budget, which is an important constraint on the amount of NO_x released from reservoir species after sunrise. The threshold revisit time requirements of 2 hours are mainly related to the diurnal cycle of air pollution levels as well as the short timescales of the mixing and chemical processes in the planetary boundary layer.

The understanding of long-range transport of pollutants requires global observations on: CO, NO_x, NO_y, O_3, aerosol optical depth, aerosol type, POPs, and Hg. Distinction between boundary layer and free troposphere would be desirable, although the threshold requirement for the satellite observations related to long-range transport are on the tropospheric column (in combination with an averaging kernel). The assumption is that the height at which transport takes place can be traced from the model's meteorological information.

The trend of tropospheric ozone and methane requires accurate monitoring of the tropospheric ozone profile and methane surface concentrations.

For source attribution the requirements are on aerosol observations and aerosol and ozone precursor observations, including SO_2, NO_2 and CO. Formaldehyde is required because it will contain important information to constrain the VOC emissions.

The aerosol requirements on the satellite observations are on the aerosol optical depth and the aerosol type, with a target to distinguish between aerosols in the boundary layer and free troposphere and a threshold for the total tropospheric aerosol optical depth. The required uncertainty (0.05) is expressed in absolute terms and based on different earlier assessments. The aerosol types to distinguish include at least standard categories such as sulphate, dust, sea salt, organic carbon (OC), black carbon (BC), and mixed aerosol. The requirement on aerosol type is that misassignments should be limited to less than about 10% of the cases.

Note that satellite NO_2 measurements are assumed to suffice to constrain NO_x emissions and NO_x ambient levels. This assumption sets some basic requirements on the chemical scheme that is to be used in the Air Quality model for the NO/NO_2 conversions.

Separate measurements of the isotopes (12C, 13C, 14C) of C for CO (and possibly CH_4) could be useful, both satelliteborne and ground-based to distinguish between, e.g., fossil fuel and biomass burning emissions.

A representative ground network is needed for the validation of the Air Quality models and the satelliteborne observations. Surface concentrations typically suffice. Additional measurements of boundary layer profiles (Lidars, Towers) at specific sites woulc be useful to validate boundary layer mixing processes in the models.

Satelliteborne estimates of the spectral actinic flux profile, necessary to determine photodissociation rates, would be desirable, especially in combination with validation of the surface level actinic fluxes using a representative surface network of UV radiation measurements. Methods exist to translate spectral UV irradiance measurements into spectral actinic fluxes. The most relevant spectral range is the 280-420 nm spectral region as the most important photodissociation reactions are limited to this range. The required spectral resolution is typically ~5 nm.

Auxilary Data Requirements

Air quality forecasting heavily relies on the combination of ground-based observations, air quality models and satellite data. The main auxiliary requirement is therefore on the availability of state-of-the-art air quality forecast model making use of analysis fields of numerical weather prediction models, detailed emission databases (both natural and anthropogenic), adequate chemical schemes and detailed descriptions of surface-atmosphere exchange processes.

2.5 Theme C: Climate

2.5.1 Protocol Monitoring and Treaty Verification

Relevant species and processes

Within the climate theme the main drivers for protocol monitoring are the UNFCCC and the resulting Kyoto Protocol (for CO_2, CH_4, N_2O, HFCs, PFCs and SF_6), as well as complementary regulations related to EU climate policy (Climate Change Committee), see Table 1. The user requirements include the monitoring of the total abundances and global concentration distribution of the radiatively active gases and aerosols as well as the detection and source attribution of the related emissions. Typically, monthly mean values are needed. It would be highly desirable to be able to derive yearly trends in concentrations and emissions within a time frame of a decade or less.

Several of the regulated greenhouse gases are 'well-mixed', i.e., their abundance in the troposphere and lower stratosphere is almost uniform over the globe. Good examples include the gases SF_6, CF_4, HFCs (HFC-134a is the most abundant), and CFCs (CFC-11 and CFC-12 are the most abundant). The atmospheric residence time of these gases is very long compared to the mixing time scales of the troposphere (typically in the order of months to one year). However, continuing but unevenly distributed emissions will maintain a latitudinal gradient and a global trend. Possible future changes in the zonal distribution of emissions, e.g. from mid-latitudes to (sub-)tropical latitude bands, may affect the latitudinal gradient. Inverse modelling can be used to trace the latitudinal concentration distribution of well-mixed gases back to latitudinal emission distributions. The applicability of inverse modelling for verification purposes was analysed recently in quite some detail in an inverse modelling workshop at Ispra (Bergamaschi et al. (ed), Inverse modelling of national and EU greenhouse gas emission inventories – Report of the workshop "Inverse modelling for potential verification of national and EU bottom-up GHG inventories" under the mandate of the Monitoring Mechanism Committee WG-1, 23-24 October 2003. JRC, Ispra, pp.144, EUR 21099 EN / ISBN 92-894-7455-6).

HCFCs (of which HCFC-22 is the most abundant) are not inert in the troposphere. Therefore, the column data of these compounds will contain, additional to latitudinal gradients, variability due to atmospheric transport. Also the columns of N_2O and CH_4, and to a lesser extent, CFCs and CO_2 will contain variability introduced by transport, mainly in the stratosphere. Clearly, dynamically-induced variabilities need to be corrected for before the column data of these gases can be used in addition to the surface measurements for the inverse modelling of emissions (see section 5.1.3).

CO_2 and CH_4 are also often referred to as 'well-mixed', however these gases are not completely inert in the planetary boundary layer and have large and variable natural sources and sinks, next to their anthropogenic emissions. For this reason the concentration distribution of these gases show more spatial and temporal variability in the troposphere. Especially for CO_2 there is a strong diurnal cycle in the planetary boundary layer, mainly due to the respiration and photosynthesis of the vegetation. Natural CH_4 emissions (mainly from wetlands) are very uncertain, but the available observations also suggest large variability. Also anthropogenic CH_4 emissions are assumed to be more variable than anthropogenic CO_2 emissions, e.g., agriculture (rice paddies, ruminants), landfills, coal mining and related to fossil-fuel production.

Ozone and aerosols are relatively short-lived and show large variability in time and space throughout the atmosphere. For the ozone radiative forcing we should further make a distinction between tropospheric and stratospheric ozone as changes in their distribution and their trends have very different origins. Stratospheric ozone is expected to recover in the coming decades (see the Ozone Layer theme), in response to the measures taken on the emissions of halogenated compounds. Although a potent greenhouse gas tropospheric ozone is nowadays mainly subject to air quality regulations (see the Air Quality theme). Ozone is not emitted but photochemically produced in the atmosphere. The two major precursor gases for tropospheric ozone are NO_2 and CO (next to CH_4 and non-methane hydrocarbons). It is anticipated that especially the NO_x and CO emissions may become subject to regulation in the future if climate policy measures are to be taken to reduce the radiative forcing by tropospheric ozone. NO_2 and CO are both short-lived and therefore show large variability throughout the troposphere.

For the direct effect of tropospheric aerosols on climate the aerosol radiative properties are crucial, especially the aerosol extinction ('cooling') and aerosol absorption ('warming') optical depth. Large volcanic eruptions can inject large amounts of aerosol into the stratosphere with can also have considerable climate effects over prolonged periods of time.

Measurement Strategy and Data Requirements

A representative surface network with stations in different latitude bands separated by ~10 degrees latitude will be well suited to monitor (changes in) the latitudinal gradient and trend of well-mixed gases. The monitoring at a certain station should include a surface concentration representative for the tropospheric background abundance in the latitude band, and a total column representative for the total atmospheric abundance in the latitude band. The surface concentration observations will allow to derive information on (changing) zonal monthly emission distributions and yearly emission trends using inverse modeling. The total column measurements will confirm the representativeness of the surface observations. Weekly-representative observations will typically suffice to arrive at the required monthly means for concentrations and emissions. In order to be able to derive trends over a decadal time frame the uncertainty on the individual observations should be very small. It is estimated that about two percent uncertainty for weekly-representative surface-based observations would typically suffice in this respect. Enhanced sampling, e.g. hourly or daily observations, can also help to reduce the uncertainties. The network should measure the regulated gases, including CO_2, CH_4, N_2O, SF_6, CF_4, HFCs, and (H)CFCs. A high-density surface network is needed to derive emissions on a country-by-country basis, typically one station every 10000-100000 km^2 and with at least one station per country. This would be very valuable. Sites should be close to emission regions for this purpose.

For CO_2 and CH_4 the global yearly trend in concentrations and emissions, and the zonal distribution of the abundance and (monthly) emissions can be obtained from a representative surface network as explained above. However, zonal distributions are of limited use for protocol verification. In order to better separate the variable natural emissions from the (more constant, although likely increasing) anthropogenic emissions, additional information on the spatial concentration- and emission distribution may be derived from satelliteborne observations. The same is true for the CO and NO_2 concentrations and CO and NO_x emissions. Although tropospheric profile information with global coverage will likely be optimal to constrain emissions, tropospheric columns or total column, in combination with an averaging kernel, with horizontal resolutions of 10x10 km^2 (target) to 50-50 km^2 (threshold) are estimated to contain sufficient information to improve upon emission estimates from surface networks alone and especially help to improve emission estimates on country-by-country basis, such as typically required for the protocols.

From available results on inverse modelling we have estimated the required uncertainty for satelliteborne CO_2, CH_4, CO and NO_2 column observations in order to be useful for improved emission estimates. The uncertainty of an individual CO_2 column retrieval on the given horizontal resolution and with 6 to 12 hours revisit times (to capture the diurnal cycle) typically needs to be better than ~0.5% with sensitivity to the planetary boundary layer. For the CH_4 columns we estimate, on the same horizontal resolution, but with only 1-day to 3-days revisit time (to capture the synoptic variability), that the uncertainty of an individual retrieval needs to be better than ~2% with sensitivity to the planetary boundary layer. For the much more variable CO columns we estimate that ~25% uncertainty would suffice, while for NO_2 columns we arrive at an maximum absolute uncertainty of $\sim 1.3 \cdot 10^{15}$ molecules cm^{-3}. The latter requirement in absolute terms implies that satelliteborne observations of the variations in the background NO_2 concentrations are not considered relevant.

By assimilation of sufficiently long and homogeneous time series possible biases in the satellite columns can likely largely be accounted for by analysis of the observation minus forecast fields, especially in combination with the assimilation of the observations from surface networks. Further, if needed to reduce uncertainties, combinations of independent observations over a certain region and/or time period can be made to retrieve emissions over longer periods (e.g. months to years) and/or larger regional domains (e.g. continents). Crucial for the CO_2, CH_4, CO and NO_2 column observations is the requirement for sensitivity to the planetary boundary layer in order to be able to relate column variability with emissions. If the columns would reflect mainly the variability in the free troposphere, the inverse modeling is very much less constrained and emission estimates are likely limited to values representative for (very) large regions or hemispheres.

Tropospheric ozone, CO, NO_2 and aerosols are short-lived and show variability in time and space to an extent that cannot be captured by surface-based networks or in-situ observations and thus their global distribution is best monitored by satelliteborne observations. However, a distributed surface network is needed for the validation of the satelliteborne measurements, either columns or profiles. Satelliteborne tropospheric profiles should have at least ~5 km vertical resolution in order to contain at least two points outside the tropics and three points within in the tropical troposphere.

Monitoring of the height distribution of tropospheric aerosols from satellite is considered of minor relevance for climate monitoring, except to distinguish between tropospheric and stratospheric (volcanic) aerosols. For the inverse modelling of aerosol emissions the data requirements are comparable to those for NO_x and CO emissions, i.e., total aerosol optical depth on similar horizontal resolutions and with a revisit time between 6 hours (target) to 3-days (threshold). The shortest revisit time would be needed to include monitoring of dust storms with very-short lived large aerosol particles.

For the selection of ozone depleting halogen compounds we have limit the requirements in the tables to the three Montreal gases that are responsible for the majority of climate forcing by halogenated compounds (CFC-11, CFC-12 and HCFC-22).

Auxilary Requirements

For long-term monitoring of the three-dimensional state of the atmospheric composition it is considered essential to assimilate the available observations in an atmospheric-chemistry numerical transport model in order to make optimal use of the available meteorological information. Furthermore, the (institutional) users will prefer complete, gridded and validated data sets with well-established uncertainties in terms of accuracy and possible biases. These requirements can be best fulfilled by an assimilation system, e.g. by systematic analysis of observation minus forecast error fields. Cross validation between different data sets will be facilitated by an assimilation system.

In the case of using column observations to retrieve emissions the aid of a numerical transport model is also needed in order to be able to correct for dynamically-induced column variabilities that should not be related to emissions.

Another important requirement for inverse modelling of emissions is the availability of a priori emission distributions, both for the anthropogenic and the natural emissions. These inventories do exist and are widely available. Nevertheless, the spatio-temporal patterns of these inventories may still be very uncertain in many cases.

2.5.2 Near-Real Time Data Requirements

Relevant Species and Processes

Climate monitoring relies to a large extent on the numerical weather prediction centres, and especially on the reanalysis projects that these centres perform. For various reasons it would be impracticable if the assimilation of atmospheric composition data by NWP centres would be limited to reanalyses projects and would be excluded from the near-real time processing. NWP centres also do not have the resources to maintain different systems. Moreover, it also could lead to inconsistencies between different model versions. Therefore, in order to improve climate monitoring it is most advantageous to include atmospheric composition observations in near-real time in the operational assimilation system of the NWP centres.

Driving the near-real time data requirements for the climate theme is therefore the assimilation of atmospheric composition observations in numerical weather prediction (NWP) models in order to improve the analysis of the physical coupled-climate system. Depending on the improvement of the analyses also improvement of the weather forecasts can be envisioned, although atmospheric composition typically impacts the atmosphere most on the longer, climatic time scales.

In addition to climate monitoring, a service to make near-real-time data sets quickly available to NWP and climate research centres will allow a continuous process of validation of the latest NWP and climate models for present-day atmospheric conditions. Near-real-time validation of adjustments in NWP models is crucial to the NWP centres. Also the capability of a climate model to simulate the latest changes in the atmospheric state is generally considered as an important model requirement to gain confidence in its ability to simulate future climate change.

In order to justify the efforts it is required that atmospheric composition data that are intended for assimilation in NWP models should have a non-negligible impact on the model simulations. Here, two types of contributions can be distinguished: a direct impact of the atmospheric composition observations on the physical climate system, e.g., stratospheric ozone largely determines stratospheric heating rates; and an indirect impact by improving the application of other available observations. One example of the latter effect is the impact of atmospheric composition on model simulated radiances, e.g. to constrain the temperature profile retrieval or the outgoing long-wave radiation at the top of the atmosphere.

The most important chemical species for NWP is water vapour. Water vapour plays a central role in the atmosphere, e.g. in the atmospheric radiation and energy budgets, in the hydrological land-ocean-atmosphere system and in several parameterisations such as for convection and precipitation formation. Accurate profiles of water vapour are needed in NWP models, throughout the troposphere and also in the lower to middle stratosphere.

In the planetary boundary layer atmospheric composition impacts on the atmospheric absorption with the largest contributions coming from aerosol absorption, water vapour, CO_2, and ozone. Also the scattering of solar radiation by aerosol particles has significant effect on how the physical climate manifests, e.g. on surface temperature and incident solar radiation. Aerosols also impact on several other remote sensing observations and improved characterisation in NWP models will reduce uncertainties related to aerosol correction.

In the free troposphere the same components as in the PBL are relevant for NWP, although the effect of the spatial and temporal variability in CO_2 is probably negligible in the free troposphere and only long-term trend monitoring is required.

In the upper troposphere and lower stratosphere water vapour, (ice) particles including cirrus and PSCs, and ozone are impacting on the physical climate. Observations of ozone, water vapour, CO_2,

CH_4, and N_2O throughout the stratosphere are important for the radiation budget. The assimilation of radiatively active gases will improve the simulation of the local heating rates and outgoing long-wave radiation at the top of the atmosphere.

Observations of inert stratospheric tracers, e.g. SF_6 or HF, but also other tracers including CO_2, CH_4, N_2O, HDO, will help to better constrain the large-scale transport in the stratosphere. These observations will be complementary to direct observations of the wind vector, planned by, e.g., the ESA mission ADM Aeolus. Direct observations of the wind vector observations will constrain in the first place the dominant large-scale motions that are most relevant on the short-term to NWP. In addition, tracer observations will help to better constrain the residual Brewer-Dobson circulation and associated vertical and lateral motions. Tracers represent air masses and have a memory of the flow over the preceding time.

Although tracer information would be most profitable on longer, seasonal and climatic time scales, it is hypothesised that sufficiently accurate inert tracer profile measurements with the given target revisit time may also positively impact on the stratospheric dynamics on short time scales. However, because absolute tracer concentrations are being measured and mixing ratios are conserved during transport this would possibly also require accurate information on the atmospheric density profile in the stratosphere as well as information on gravity waves. At this stage it is rather uncertain what could be the impact of tracer observations for NWP on short time scales relevant to weather prediction.

It is noted that stratospheric observations of the tracers CH_4 and HDO, in addition to H_2O, can help to better constrain the stratospheric water vapour budget.

Measurement Strategy and Data Requirements

For NWP and climate monitoring applications the three-dimensional water vapour distribution in the boundary layer, free troposphere and stratosphere is required with global coverage. Therefore, an integrated approach of satelliteborne observations, a representative global in-situ network of radiosonde and surface-based remote-sensing techniques is needed, coupled with model information. Two-to-three kilometre vertical resolution for H_2O would be very advantageous, threshold for the satellite contribution is the distinction of boundary layer, free tropospheric and stratospheric water vapour sub-columns. For climate purposes the target horizontal resolution in the troposphere is about 10x10 km^2, although water vapour spatial variability is large and structures with less than one kilometre are associated with e.g. fronts. Uncertainty of column data typically needs to be better than ~5% to improve upon current modelling capabilities of weather centres. Tropospheric water vapour has a strong diurnal cycle and the required revisit time for satelliteborne observations is typically ~6 hours. The revisit time can be limited to one day to one week (threshold) in the stratosphere. Given the spatiotemporal variability in water vapour the optimal strategy to water vapour is likely combined use of ground-based systems (e.g. GPS), radio sondes, polar orbiting and geostationary platforms.

Aerosol absorption and aerosol scattering are important for the radiation budget and atmospheric corrections. Threshold requirements for operational use include the separation of the total extinction optical depth in an absorption and scattering contribution. Distinction between boundary-layer, free-tropospheric, and stratospheric aerosol would be advantageous, as well as further aerosol characterisation, in particular the aerosol phase function given the important radiative effects of aerosols. The same set of requirements applies to cirrus and PSC ice particles (optical depth, phase function) albeit limited to the higher altitudes. Spatial scales for aerosol are typically comparable to water vapour. Revisit times for tropospheric aerosols can typically be limited to about one (target) to a few days (threshold) and to a couple of days to a week in the stratosphere.

Ozone profile information is most relevant in the stratosphere and upper troposphere where the (variation in) ozone radiative forcing is most effective. Tropospheric ozone threshold requirements are limited to column observations (in combination with an averaging kernel), while distinction between the boundary layer and free troposphere would be advantageous. In the UTLS region, co-located profile observations of O_3 with both HNO_3, HCl and/or CO are desirable to help to constrain stratosphere-troposphere exchange processes. Hereto, the observations need to be both rather accurate and have high vertical resolution (1 km target, 3 km threshold).

In-situ CO_2 observations in the PBL and total column CO_2 observations can be obtained from a surface network. Satelliteborne CO_2 column observations (in combination with an averaging kernel), if sufficiently accurate to include the naturally occurring column variability that is caused by the diurnal respiration of the vegetation, can help to provide global coverage. The column data need to be sensitive to the planetary boundary layer. A representative surface network would be needed for validation and corrections of possible biases.

As explained in the former section tracers can constrain the stratospheric circulation. Suitable candidates are inert gases as SF_6 and HF, but other long-lived compounds such as CO_2, N_2O, CH_4 and HDO can be used as well. Typically a tracer that can be observed most accurately need to prevail. The required uncertainty is directly related to the gradient over the specified spatial resolution (100-200 km horizontally, 1-3 km vertically). Target revisit times are about 12 hours. With the threshold revisit time of one week only information on the circulation on seasonal to multi-annual time scales will be obtainable.

For the radiation budget stratospheric profiles are required for the radiatively active gases H_2O, O_3, CO_2, CH_4 and N_2O. The stratospheric water vapour budget can be constrained by measurements of H_2O, HDO and CH_4. Profiles are needed with three-to-five kilometre vertical resolution throughout the stratosphere.

Finally, near real time data delivery for this application implies that the data needs to be available to an operational modelling environment within a couple of hours after observation. In that case a significant part of today's observations can still be used for the analysis of the day.

Auxilary Data Requirements

The main users for near-real time data within the climate theme are the NWP centres. These centres need near-real-time information on numerous aspects of the land-atmosphere-ocean-cryosphere system that all contribute to the analysis of the atmosphere and therefore to the initial state on which the weather prediction is based, and on which climate monitoring relies. Atmospheric composition is one of the key elements for the monitoring of the climate system.

2.5.3 Assessment

Relevant Species and Processes

Within the Climate theme the operational data requirements for understanding need to be based on long-term science questions relevant to understand the interactions between atmospheric composition and the physical climate. The relevant issues are typically addressed in the regular IPCC scientific assessments.

Important science questions that require long-term operational monitoring are related to:

- Understanding of the radiative forcing of climate and the changes in forcing over time, including possible volcanic eruptions, and also including the forcing of climate on local to regional scales

- Understanding of the abundance, evolution, and, if relevant, spatial distribution of the forcing agents
- Understanding of the stratospheric water vapour budget and the monitoring of the water vapour trend in the UTLS and above.
- Understanding of the role of the ozone layer evolution on climate change
- Understanding of the role of possible changes in the ***Brewer-Dobson circulation*** on climate change, including possible changes in the position and strength of the polar and sub-tropical jets, changes in the position and strength of the inter-tropical conversion zone (ITCZ) as well as changes in the mesosphere (air density)
- Understanding of the role of long-term changes in the oxidising capacity of the troposphere for its effect on the atmospheric residence time of the climate gases
- Concentration monitoring for the detection and attribution of long-term changes in the natural as well as anthropogenic emissions of the forcing agents and their precursors

Data requirements related to the understanding of the role of atmospheric composition changes for climate similar detailed requirements have been laid down in the ACECHEM mission proposal and the report of the preceding ACE requirements study [RD10]. The reader is referred to these documents for additional scientific background.

Measurement Strategy and Data Requirements

The processes underlying the interactions between climate change and atmospheric composition change are typically rather slow (months, years, decades) and therefore can only be better understood by increasing the amount of available long-term and homogeneous data sets on atmospheric composition. Although global coverage is required for most observations, the Upper Troposphere-Lower Stratosphere (UTLS) layer it probably the most important atmospheric domain because it is both chemically and radiatively very active. However, other atmospheric layers are relevant as well, e.g. the long-term trend in stratospheric water vapour is badly understood and this needs to be monitored by long-term accurate global-scale profile measurements including the stratosphere above the UTLS layer. Profiles of H_2O, HDO and CH_4 are needed with three-to-five kilometre vertical resolution. Column data can be useful and should be given in combination with an averaging kernel. For the radiation budget vertical profiles are required for the radiatively active gases H_2O, O_3, CO_2, CH_4 and N_2O in both the UTLS and the overlying stratosphere. Tracer measurements to constrain the Brewer-Dobson circulation also need to extent over the full stratosphere, and possibly should even include parts of the mesosphere. Changes in the mesosphere, e.g., in air density could give also indication of temperature changes in the middle atmosphere. Suitable tracer candidates for diagnosing the Brewer-Dobson circulation are typically inert gases such as SF_6 and HF, but other long-lived compounds such as CO_2, N_2O, CH_4 and HDO can be useful as well. Likely the tracers that can be observed the most accurately need to prevail.

Atmospheric composition related climate processes in the troposphere include, e.g., gaseous and aerosol absorption and aerosol scattering in the PBL, secondary aerosol formation relevant for cloud formation, aerosol deposition on ice surfaces affecting the ice surface albedo and oceanic dimethylsulfide (DMS) also affecting cloud condensation nucleii.

In-situ observations in the UTLS by operational aircraft measurements will be useful in addition to satellite measurements and should include preferably O_3, CO, NO_y (or HNO_3), NO_x, HCl and H_2O. The airborne measurements can especially help to better constrain stratosphere-troposphere exchange as well as chemical processes

Surface-based atmospheric composition measurements contributing to understanding of climate are most relevant to monitor the long-term evolution in the long-lived gases. In addition the networks are crucial for the validation of the global-scale satellite measurements. The need for a detailed knowledge on the 3-D water vapour distribution and its changes over time would be improved by surface-based networks such as the radiosonde network and GPS-based configurations. The monitoring of the 3-D distribution of ozone and aerosols would be improved by surface based monitoring of surface concentrations and total columns as well as a network of profile measurements of sondes and LIDARs.

Auxilary Data Requirements

Climate research centres need long-term information on numerous aspects of the land-atmosphere-ocean-cryosphere system that all contribute to the analysis of the climate system. Atmospheric composition is only one component of the Earth System. The usefulness of atmospheric composition data for the study on climate change will partly depend on the information that will be available for the other components of the Earth System.

3 Assessment of Existing and Planned Satellite Misssions and Ground Networks

3.1 Outline and Context

In this chapter the capabilities of existing and planned missions and networks are examined and assessed against data requirements, defined previously within the study. The performance of specific atmospheric sounding instruments has been assessed in terms of their height-coverage, precision and vertical resolution, horizontal and temporal sampling, and then compared to the quantitative requirements.

Instrument descriptions, and references to further details, are provided, followed by assessments of instrument capabilities versus requirements. An analysis in terms of satellite missions, comprising one or more instruments, is also presented.

To set the context for the space-borne elements a review of future programmes, relevant to atmospheric sounding, by European and other national agencies is included. The data requirements in this study are defined for longer term "monitoring" purposes. In this context the operational satellite observing system, comprising the European MetOp and the American NPOESS missions, is the foundation, and therefore merits particular attention.

3.2 Programmes of ESA, Eumetsat and National Space Agencies for Future Atmospheric Sounding Missions

European, American and national agencies are continuously developing new space programmes. The current status, with relevance to atmospheric sounding, is summarised in following sections. The programmes include both research and operational missions. In the contex of this study the latter are more directly relevant although the research programmes will, no doubt, contribute significantly to development of new, advanced sensors.

3.2.1 ESA Explorer Programme

There are six approved missions within the ESA Explorer programme:

- CryoSat - to measure polar marine and continental ice (2005)
- GOCE - Gravity field and steady-state Ocean Circulation Experiment (2006)
- SMOS - Soil Moisture and Ocean Salinity mission(2007)
- ADM-Aeolus - Atmospheric Dynamics mission (2007)
- Swarm - to survey the geomagnetic field and its temporal evolution (2009)
- Earth-CARE - to quantify aerosol-cloud radiation interactions (2012)

In ESA's currently open Call for Ideas for future Explorer missions, there are three identified priority areas:

- Global water cycle
- Global carbon cycle
- Atmospheric chemistry and climate.

Attention is also drawn to the human element and its impact on these three priority areas. The schedule identified in the Call for Ideas indicates selection by end of 2005 of six candidate missions for pre-Phase A study, from which up to three would subsequently be selected for Phase A study and, finally, one would be selected in 2008 for Phase C/D implementation and launch after 2012.

Decisions on the next cycle of Explorer mission(s) will be informed and influenced by those already made and still to be taken on the GMES Sentinel Programme and by other Agencies on their own future programmes, notably Eumetsat and national agencies within Europe and the US ESSP and NPOESS programmes.

3.2.2 ESA/EU GMES Sentinel Programme

The GMES programme is intended to establish and develop applications (other than NWP) for operational usage of satellite EO data. The initial phase is to demonstrate user applications and services based on satellites which are currently operational (eg ESA's ERS-2 and Envisat). This includes the GMES Service Element Atmospheres Project: PROMOTE. The next phase is to define, develop and implement new space missions, the so called Sentinels, which are primarily intended to serve the future needs of operational users. The current status is that definitions of three Sentinel missions to monitor, ocean and land surface properties, have reached the necessary level of maturity for ESA to commission Phase A studies. An ESA study to support the definition of a Sentinel mission to monitor atmospheric composition is due for completion in mid-2005, and recommendations from this study, along with findings from the first phase of the PROMOTE project, will inform ESA's mission specifications for Phase A studies due to be launched early in 2006.

The needs of the European met services for satellite and other atmospheric data for numerical weather prediction are served by Eumetsat. Although the current generation of operational satellites in polar (MetOp/EPS) and geostationary (MSG) orbit were designed primarily to meet these needs, they include several instruments which measure atmospheric constituents additional to the needs of NWP. Eumetsat has acquired a mandate within Europe to facilitate satellite measurements to monitor climate and is also seeking to broaden the range of operational applications it supports, e.g. to include air quality forecasting, in its future programme post-MSG and -EPS.

In regard to monitoring of atmospheric composition in particular, there currently appears to be potential overlap in scope between the EU/ESA Sentinel programme and the Eumetsat post-MSG and post-EPS programmes.

3.2.3 Eumetsat post-MSG and -EPS Programmes

Meteosat 2nd Generation has been operational for over one year and the first of three MetOp/EPS platforms is due for launch in 2006 into a sun-synchronous polar orbit with ascending node equator crossing time of 21:30. These operational systems have been designed to provide data to the met services until ~2015 and ~2020, respectively. However, Eumetsat is already taking initiatives to define the successor geostationary and polar orbiting missions. The heritages for both will draw heavily from MSG and MetOp, not least because the met services currently anticipate that observational requirements for NWP are not likely to change radically during the next fifteen years. With the likelihood that reciprocal agreements with US data providers similar in kind to those in place for exchange of data between NOAA and MetOp satellites would be negotiated for future operational systems, it can be envisaged that US plans for the implementation and future evolution of NPOESS will heavily influence Eumetsat decisions on its polar orbiting system post-EPS, and likewise Meteosat 3rd Generation.

Eumetsat recently commissioned a study to explore whether MSG SEVIRI measurements in the 9.7 µm O channel could add value to those from GOME-1 in polar orbit. The findings will inform future decisions by Eumetsat in regard to instrumentation for MTG. The utility of data from polar orbiters with different equator crossing times will be explored as they become operational in ESA's GMES Service Element Atmospheres Project PROMOTE. This will inform future decisions by Eumetsat in regard to configuration of a post-EPS system.

3.2.4 NASA ESSP

Following on from the Terra, Aqua and Aura missions, NASA's Earth System Science Pathfinder (ESSP) programme currently comprises six missions:

- GRACE - Gravity Recovery and Climate Experiment (2002)
- CALIPSO - Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (2005)
- Cloudsat - to measure cloud vertical structure (2005)
- OCO - Observing Carbon Observatory (2007)
- Aquarius - to measure sea-surface salinity(2008)
- HYDROS - Hydrosphere State Mission to measure soil moisture (2010)

It is anticipated that a call for the next ESSP mission may be issued later this year in co-ordination with ESA. The scope of this next call is not known at present.

3.2.5 NASA Instrument Incubator Programme

This NASA programme fosters development of innovative remote-sensing concepts and the assessment of these concepts in ground, aircraft, or engineering model demonstrations. It is intended to provide a continuing source of mature instrument designs, merging state-of-the-art technologies with measurement objectives, available for use in the next generation of Earth science missions. Preparatory activities directed towards a variety of future atmospheric sounding instruments are in progress.

3.2.6 NPOESS - National Polar-orbiting Operational Environmental Satellite System

During the next two decades the US is planning to launch a series of six operational satellites into three different sun-synchronous polar orbits, to serve the needs of NOAA and other US government departments. Ahead of this, a demonstrator of advanced instruments is due for launch through the NPOESS Preparatory Project (NPP) in 2006.

Planning of the NPOESS system takes MetOp into account explicitly, reflecting the reciprocal agreement for data exchange between NOAA and Eumetsat to facilitate numerical weather prediction. Initial enquiries indicate that it would be reasonable to assume that access of European users to data from NPOESS (including NPP) will also be approved for research purposes and also potentially for operational uses other than NWP. This leads to the important conclusion that the Eumetsat programme post-MSG and -EPS and an EU/ESA Sentinel mission to monitor atmospheric composition should be defined so as to complement/supplement and not to replicate NPOESS.

Within the NPOESS suite, the following sensors have been designed to deliver atmospheric data:

- VIIRS - Visible/Infrared Imager/Radiometer Suite
- CMIS - Conical Microwave Imager/Sounder
- CrIS - Cross-track Infrared Sounder
- OMPS - Ozone Mapping and Profiling Suite
- APS - Aerosol Polarimeter Sensor
- ATMS - Advanced Technology Microwave Sounder
- ERBS - Earth Radiation Budget Sensor
- TSIS - Total Solar Irradiance Sensor

However, although VIIRS and CMIS are slated to fly on all NPOESS platforms, other relevant sensors will not fly in the 21:30 ascending node equator crossing time. CriS. ATMS and OMPS will be deployed on two consecutive platforms to be launched with the following equator crossing times:

- CrIS & ATMS: 13:30 & 21:30
- OMPS: 13:30.

With MetOp scheduled to occupy the 21:30 orbit until ~2020 some adjustment can be foreseen to avoid redundancy with NPOESS during this period.

3.2.7 Other National Agencies

JAXA

ISS JEM-SMILES

The Japanese National Institute of Information and Communications Technology NICT (formerly CRL) are responsible for the SMILES (Superconducting Submillimeter-Wave Limb-Emission Sounder) on JEM (Japanese Experimental Platform), the first space-borne SIS receiver which is cooled to 4K by LHe cryostat. The target species in the 640 GHz frequency band include molecules with very faint emission lines e.g. BrO and ClO, detectable with Tsys 500K, as well as O and HCl. The instrument also features other novel technology. Plans are for SMILES to operate for one year on the ISS following launch in 2007.

GOSAT - Greenhouse gases Observing SATellite (2007)
Following TRMM, ADEOS-II and earlier missions, JAXA is now developing an Advanced Land Observing satellite (ALOS) and GOSAT.
Building directly on the heritage from its successful earlier mission Interferometric Measurement of Greenhouse gases (IMG), JAXA is now planning to launch a nadir-viewing FTIR spectrometer to target CO and CH . This would complement, to some extent, NASA's OCO mission, which has the same mission objective and is scheduled for launch on a similar time-frame but which would utilize a grating spectrometer to measure backscattered solar radiation at near-IR wavelengths instead of an FTS to measure upwelling thermal emission at mid-IR wavelengths.

CNES

CNES has developed a variety of sensors for land surface, oceanic and atmospheric observations and retains active involvement in the development of advanced instruments, both passive and active. However, following launch of PARASOL in December 2004, CNES does not currently have a formal commitment to lead any specific future atmospheric sounding mission. Building directly on heritage from earlier French ground-based and airborne FTIR instruments and, notably, the Infrared Atmospheric Sounding Interferometer (IASI), which CNES has supplied for the three MetOp platforms, alternative concepts are being studied for an advanced FTIR instrument in polar (TROC) or geostationary (GeoFIS) orbit.

NIVR

NIVR developed the OMI instrument for NASA's Aura mission and previously contributed near-IR detectors to the SCIAMACHY instrument for ESA's Envisat. Several new concepts for atmospheric sounding from polar orbit are under study in the Netherlands. These include an advanced uv/vis grating spectrometer (direct heritage from OMI) with spectral coverage extended into the NIR and SWIR (heritage from SCIA) to sound tropospheric trace gases. A second concept under study is that of a multi-angle polarising imager to sound tropospheric aerosol.

ASI

ASI has led earlier studies of a Radiation Explorer in the Far InfraRed (REFIR) and could pursue this concept in future.

DLR

Following selection of two candidate missions for its future national programme, both of which target Earth's surface properties, it appears unlikely that DLR could initiate or contribute German national funding towards an atmospheric sounding mission within the next decade.

SNSB/CSA

SNSB is lead agency for the Odin mission, which recently completed its fourth year of operations. In collaboration with France and Germany, Sweden developed the Sub-Millimetre Radiometer (SMR) for limb-sounding stratospheric trace gases of importance to ozone chemistry, along with the associated ground processing system. CSA supplied the Optical Spectrograph and Infrared Imaging System (OSIRIS) to the Odin mission for limb-sounding of stratospheric trace gases and aerosols and the Measurements Of Pollution in The Troposphere (MOPITT) instrument, an IR gas-correlation radiometer, to NASA's Terra mission. In 2003, CSA successfully deployed SCISAT which comprises ACE-FTS and MAESTRO, solar occultation instruments observing at IR and uv/vis/nir wavelengths, respectively. CSA is now developing a new hyperspectral imager (HERO).

STEAM/SWIFT

Following on from Odin, a renewed partnership between SNSB and CSA has now been initiated to develop the (Swedish-led) STEAM mission in conjunction with CSA's Stratospheric Wind Interferometer For Transport studies (SWIFT) mission. The latter has as part of its heritage CSA's earlier instrument WINDII, which measured upper atmosphere winds from NASA's Upper Atmosphere Research Satellite for thirteen years.

3.3 Assessment of Instruments

3.3.1 Observation Techniques

Atmospheric observations can be carried by a number of techniques and from a variety of platforms. The technical note on this workpackage (WP2200) includes descriptions of instruments considered in this workpackage that are part of ground-based networks and satellite missions which are current or well-planned in the future.
The observation techniques are separated into the following categories :

- Ground Networks
    - trace gases
    - aerosol
- Satellite Observations
    - nadir-uv/vis/nir
    - passive nadir-sounding of aerosol
    - nadir-mir
    - lidar
    - limb-mm/sub-mm
    - limb-mir
    - limb-uv/vis
    - occultation

3.3.2 Instrument Data

Performance data has been collected for products that are or will be routinely provided by the instruments outlined previously. This includes:

- Horizontal resolution, horizontal sampling
- Temporal sampling, as revisit time
- Vertical resolution and uncertainty in each height range as defined in WP2100
- Author and source reference

The instrument data are from a variety of sources and the information available at different stages of maturity. Some existing instruments already produce data which has been well characterised and studied, others are still in comissioning and validation phases. The planned instruments are still to be launched and their performance can only be estimated on the basis of existing simulations or by drawing on experience with comparable instrumentation already in flight.

The approach taken for instrument data is as follows :

- Where possible, the instrument data are based on current performance from standard processing. If non-standard schemes are used these must be justified.
    - Options to revise these are only permitted on the basis of improvements to data quality which are either, already demonstrable by scientific processors, or confidently expected in future, on the basis of realistic simulations
    - For simulations convincing arguments would need to be made that the required further advances, such as the L1 data quality, are entirely realistic
- For planned missions the data provided depends on realistic simulations.

3.3.3 Analysis Method

The instrument capability data have been compared to requirements for all nine user application areas, for ground-based and space-borne instruments. Instrument assessement tables have been produced to indicate the requirement cases for which appropriate measurement data is available. These tables reflect the Data Requirement Tables provided as output from WP2100. In many instances requirements or capabilities are given as a range, so the tables indicate the different levels of possible agreement. Fields marked requirements met partially indicate that the capability matches the least demanding requirement (also referred to as "threshold"); requirements met fully means that the most stringent requirement (or "target") is met. It should be noted that:

- The instrument assessment tables are based on the Data Requirements Tables of 23 December 2004. They are intended to show how the data requirements are addressed by the current systems, not to provide a comprehensive list of the available measurements of atmospheric constituents provided by the instruments under consideration.
- In many cases the individual Data Requirement tables have been represented by a set of instrument tables on separate pages to make for easier reading. The tables are then labelled with extra identifiers in roman numerals, i, ii, iii and so on, e.g. A1G(i), A1G(ii).
- Some instruments have several retrieval methods and operating modes so can appear multiple times e.g. SCIAMACHY.
- The presence of an unfilled block may indicate that an instrument measures the target in question but not in the relevant height range.
- Some uncertainty requirements are stated for *zonal average (ZA*) and *1000 km average (1000km)* fields. In these cases the horizontal sampling numbers provided in the instrument performance data files have been used to determine the number of samplings included in the required area. Effective uncertainty has then been calculated by assuming simple averaging as , where is the number of measurements in the averaging area. This number is then compared to the requirements. The assumed area for zonal average requirements is 20000 km 110 km, approximately equivalent to a latitude band of 1° at 60° N. For the 1000 km requirement the relevant area is simply taken to be 1000 km 1000 km.

The full detail of the analysis, including a full set of tables, is presented in the technical note on this work package (WP2200). One example table, for application A2S, indicating comparison of capabilities against requirements is shown in Figures 3.1-3.3. The results have been examined for all instruments for which data was available and conclusions drawn for each application theme. For the space-based requirements capabilities have also been drawn together for existing and planned satellite payloads i.e. combinations of instruments.
It should be noted that in the written summaries the requirement categories (horizontal and vertical resolution, revisit time and uncertainty) are assessed in combination. The phrase "meets requirements" or similar means that an instrument meets the requirements in all categories at least partially.

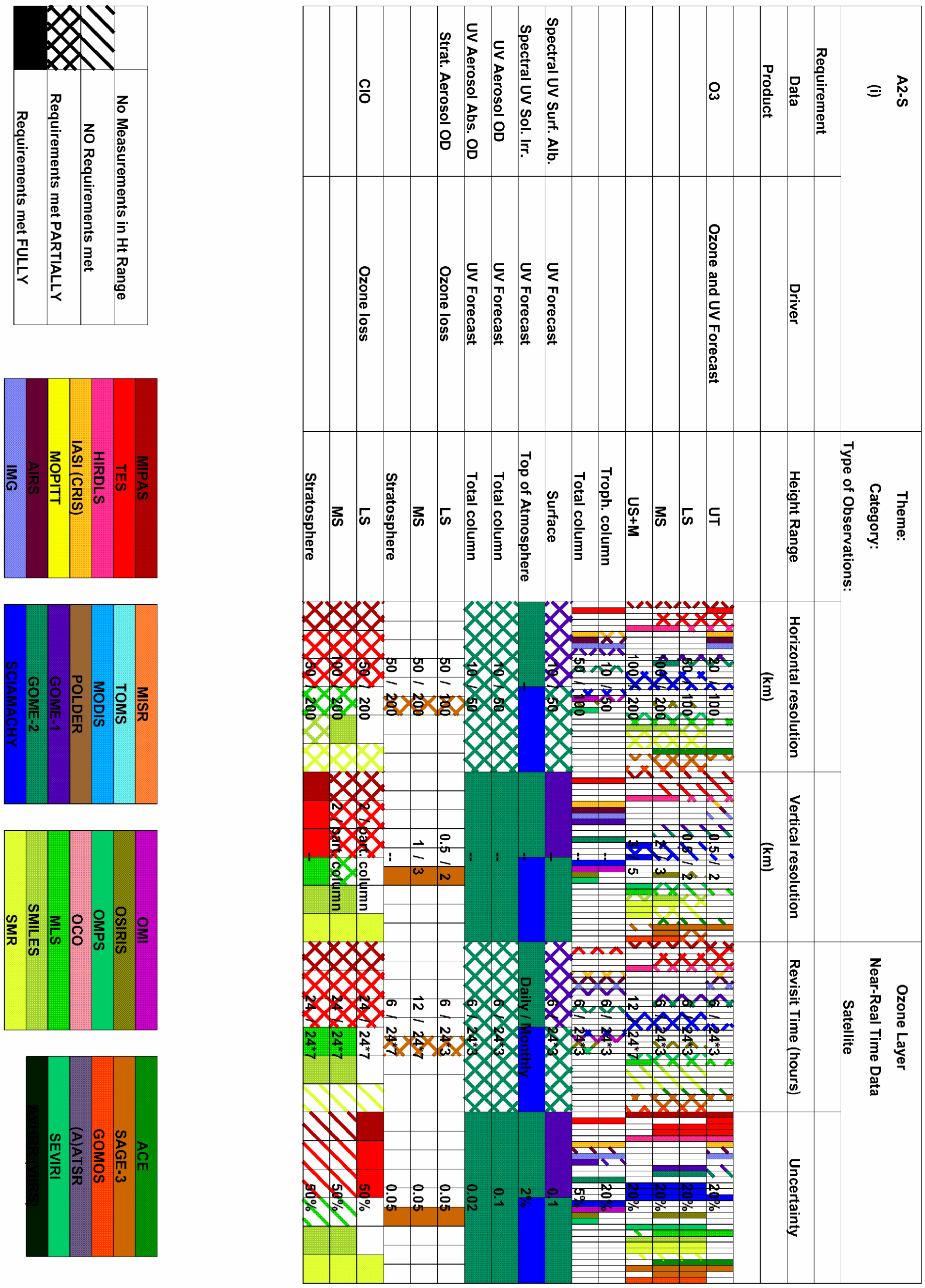

Figure 3.1. Capabilities against Requirements. Application A2. Spaceborne (part i)

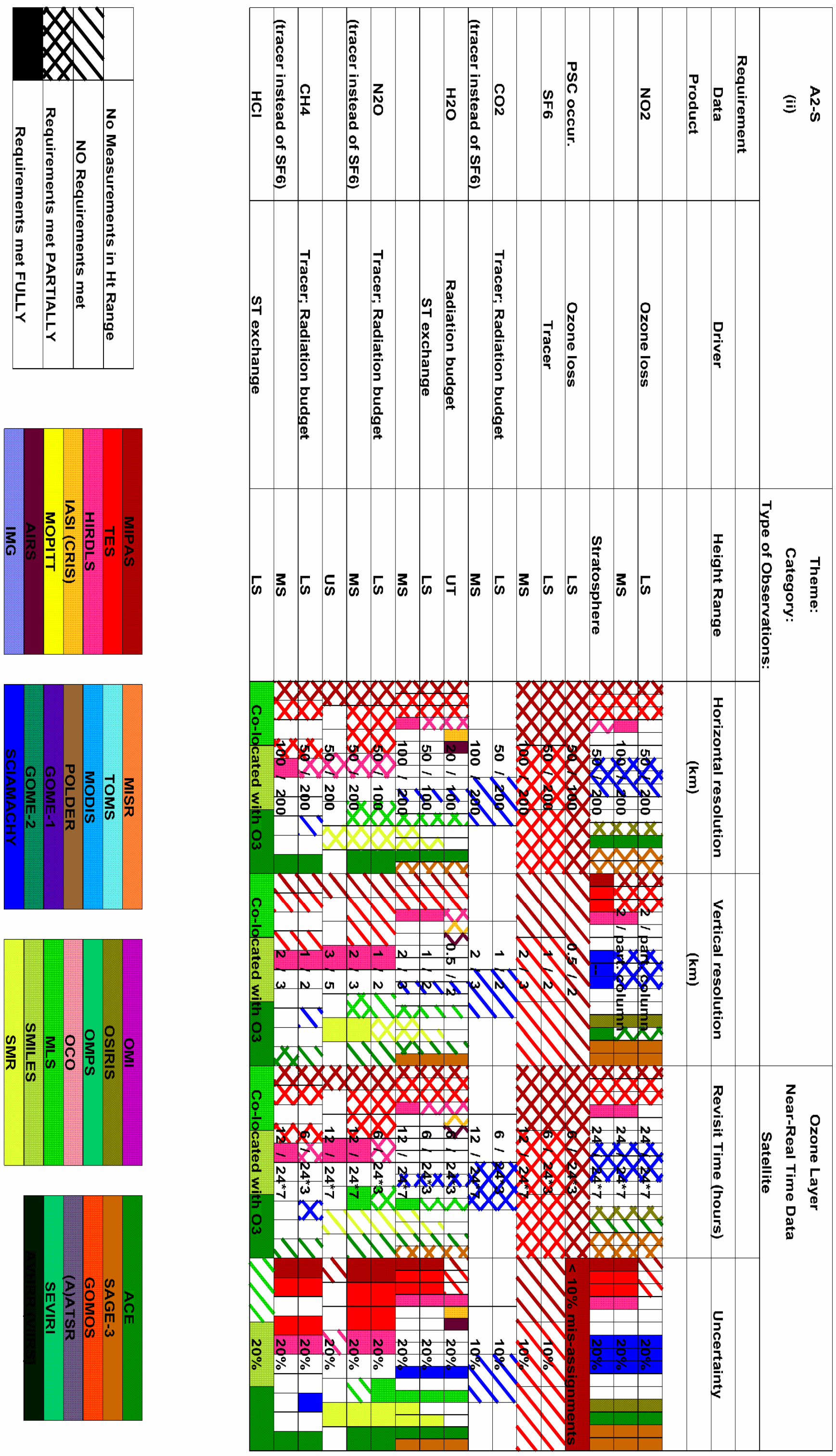

Figure 3.2. Capabilities against Requirements. Application A2. Spaceborne (part ii)

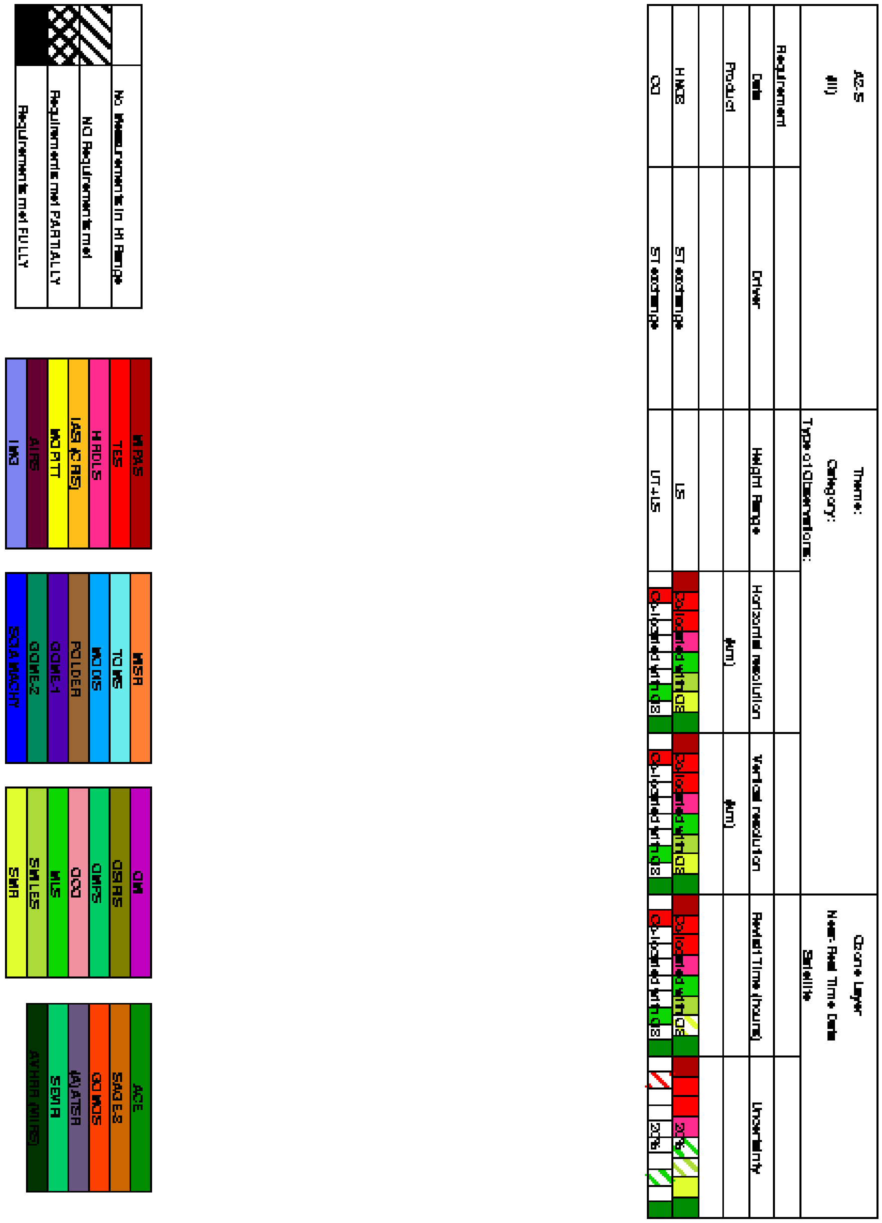

Figure 3.3. Capabilities against Requirements. Application A2. Spaceborne (part iii)

3.3.4 Summary by Theme

In this section the instrument performances are summarised for each study theme, A Ozone Layer, B Air Quality, C Climate. Summaries of findings are presented for each application area separately, i.e. 6 in each theme, and also, more generally, for each theme and instrument group, satellite and ground-based, as a whole.

Theme A – Stratospheric Ozone and Surface UVRadiation

A1S – Protocol Monitoring

- O_3 columns can be provided as required
- Measurements of UV related products can be provided.

A2S – Near-real Time Applications

- Most species measured
- Measurements of UV related products can be provided
- Vertical resolution requirements often difficult to meet e.g. 2 km in the UTLS

A3S – Assessment

- Most species measured
- Several species, especially bromine compounds, are not provided
- Measurements of UV related products can be provided
- Infrared instruments MIPAS, TES and HIRLDS often provide the only measurement capability

Comments

- HIRDLS type measurements are very useful in addressing the requirements
- MIPAS and TES often only fail the vertical resolution requirement
- Most products are available.

A1G – Protocol Monitoring

- Most species are measured, though many only at the surface by in-situ techniques
- Measured species meet the requirements
- No UV products

A2G – Near-real Time Applications

- Many measured species meet the requirements
- The required vertical resolution is not achieved in some cases
- The "tracer" species required for validation are not measured in the required manner
- No UV and aerosol products

A3G – Assessment

- Very many species in this category most of which are observed, however often only at the surface
- Measured species often fail the vertical resolution requirements

Comments

- A number of the required species are not observed
- Many measurements that are made meet the requirements, but required height ranges are often not covered

- In several cases the vertical resolution requirement is difficult to meet

Theme B – Air Quality

B1S – Protocol Monitoring

- Most species are measured in appropriate height ranges and as columns but do not meet requirements
- There are few measurements of the FT and boundary layer regions and the height-resolved measurements that do exist are not satisfactory
- Revisit time is the critical requirements

B2S – Near-real Time Applications

- Most products are measured in appropriate height ranges but do not meet requirements
- There are few measurements of the FT and boundary layer regions and the height-resolved measurements that do exist are not satisfactory
- Revisit time and horizontal resolution are critical requirements

B3S – Assessment

- Several species are measured but do not meet requirements
- There are few measurements of the FT and boundary layer regions and the height-resolved measurements that do exist are not satisfactory
- Revisit time and horizontal resolution are critical requirements
- Several required products are not measured

Comments

- There are few measurements in the FT and, particularly, the boundary layer
- Revisit time requirement is consistently not met

B1G – Protocol Monitoring

- Most products are measured at the surface and, in cases where the in-situ instruments are deployed in towers, the boundary layer is also accessed

B2G – Near-real Time Applications

- Most products are measured at the surface and, in cases where the in-situ instruments are deployed in towers, the boundary layer is also accessed
- Higher altitudes not measured with appropriate revisit time

B3G – Assessment

- Several products not measured
- Many required altitudes not measured to requirements

Comments

- Several of the required species are not observed or only at a limited number of altitudes and the measurements often do not meet the requirements

Theme C – Climate

C1S – Protocol Monitoring

- Many of the required species are measured and meet requirements in most cases

- CO_2 uncertainty requirement is difficult to meet

C2S – Near-real Time Applications

- Many tropospheric and lower stratospheric requirements are difficult to meet, e.g., O_3 and H_2O vertical resolution (2 km in the UTLS)

C3S – Assessment

Large number of required species A number of useful measurements but often not for all required altitudes Many tropospheric requirements are difficult to meet e.g. O and H O vertical resolution (2 km in the UTLS

Comments

- A large number of species are required for this theme
- Many tropospheric and lower stratospheric requirements are difficult to meet

C1G – Protocol Monitoring

- Many species are measured but requirements are not met at all altitudes
- No height-resolved aerosol products

C2G – Near-real Time Applications

- A number of the species are measured but some altitudes are not covered and there is a lack of vertical resolution in many measurements
- No height-resolved aerosol products

C3G – Assessment

- Very many species in this category many of which are not observed
- Measured products do not meet requirements in many cases and in particular for vertical resolution and uncertainty

Comments

- Several species not measured
- Lack of height-resolved measurements
- Many measurements do not achieve the required vertical resolution

Summary for Satellite Instruments

There follows a general summary for each theme with respect to satellite observations. The terms threshold and target are used to refer to the least demanding requirement and the most stringent requirement respectively.
A similar summary for ground-based measurements follows thereafter.

Theme A

Products : Several bromine compounds are not measured.
Horizontal Resolution : Generally the threshold requirements are met but improvement would be useful to come closer to target values.
Vertical Resolution : In many cases the threshold requirement, typically 3 km, is not met. Higher vertical resolution measurements would be of significant benefit
Revisit Time : Generally, the threshold requirements are met; improvement would be useful.
Uncertainty : In most case the target values are achieved.

Theme B

Products : Several compounds, including a number of nitrogen species are not provided appropriately.
Horizontal Resolution : The threshold requirements are typically achieved.
Vertical Resolution : The capabilities are generally satisfactory in this regard, although improvement is required for some profile measurements requiring 2 km resolution.
Revisit Time : The threshold requirements are, in general, not met.
Uncertainty : Requirements are only satisfactory in a few cases and improvement is required for many requirements.

Theme C

Products : Most products are measured.
Horizontal Resolution : Generally inside threshold values.
Vertical Resolution : The threshold values are achieved in many cases. For requirements of 3 km or less measurement improvements are necessary.
Revisit Time : Generally target or threshold is achieved.
Uncertainty : Target requirements are met in many cases.

Summary for Ground-based Instruments

Theme A

Products : Most products are not measured in all required height ranges. Aerosol, tracers and some organic compounds are not well addressed.
Vertical Resolution : Requirements are generally only achieved for surface measurements. In many cases only columns are provided, although height resolved profiles are also required.
Revisit Time : Target requirements are met in most cases
Uncertainty : Target requirements are met in most cases

Theme B

Products : Particulates and several organic compounds are not measured.
Vertical Resolution : A number of measurements achieve target and threshold values. Height-resolved measurements of the boundary layer are generally lacking.
Revisit Time : Generally, the threshold requirements are met.
Uncertainty : Many target requirements are met.

Theme C

Products : Most species are measured though not in all required height ranges.
Vertical Resolution : Many height ranges are not addressed and, in other cases, threshold requirements not met. For column and surface measurements the target requirements are met.
Revisit Time : Target requirements are met in many cases.
Uncertainty : Target requirements are met in a number of cases, however for several measurements the threshold requirements are not achieved.

3.4 Summary of Capabilities and Limitations

3.4.1 Capabilities of Satellite Systems

Cloud and Aerosol

Imagers on the operational satellites MSG and MetOp/NPOESS, the research satellites (ERS-2, Envisat, Terra and Aqua), PARASOL and EarthCARE and the Sentinel-3 satellite will provide geographical coverage on tropospheric cloud and aerosol, together with certain other physical properties (e.g. optical depth, size parameter, phase, liquid water content). Radar and lidar instruments on Cloudsat, CALIPSO and EarthCARE will provide vertical profile information on cloud and aerosol along the sub-satellite track, although the design lifetimes of active instruments are relatively short (~3 years). Ice water content is a significant meteorological variable but will not be determined with sufficient accuracy by the passive imagers. Visible and IR wavelengths are insensitive to the size distribution of particles in the cirrus range. Extinction efficiencies of these size components typically peak in the sub-mm or THz regions, which are not measured at all by planned missions. Nadir-viewing imagers and spectrometers offer little if any information on either stratospheric aerosols or polar stratospheric clouds.

Water Vapour / Humidity

Water vapour sounding adequate for NWP will be performed in cloud-free scenes by the MetOp/NPOESS system. The operational system will not provide useful water vapour data above the tropopause and vertical resolution in the upper troposphere will not be sufficient for some future applications.

Ozone

MetOp/NPOESS (GOME-2/OMPS) should provide adequate observations with which to monitor stratospheric and total column ozone. Tropospheric ozone retrieval has been demonstrated for GOME-1 and simulations indicate that nadir-FTIR observations from IASI/CrIS may add significant value to height-resolved O_3 information from GOME-2/OMPS in the troposphere. Ozone observations by the operational system will not have sufficient vertical resolution in the UTLS for future monitoring applications. A ground pixel size smaller than that of GOME-2 or OMPS to allow more frequent sounding of the lower troposphere between clouds would be desirable for future monitoring applications and for AQ forecasting The operational system will provide uv/vis observations at only two local times (9:30am for GOME-2 and 13:30 for OMPS). Ozone observations at additional local times might be desirable for AQ forecasting.

Trace Gases other than Ozone

MetOp and NPOESS uv/vis sensors should provide slant columns of several tropospheric trace gases in addition to O_3 , i.e. NO_2 , SO_2 , H_2CO and BrO. Nadir-observations contain no height-resolved information. Limb-observations of the stratosphere made simultaneously by OMPS will allow slant-column information from nadir-observations to be assigned to the troposphere. For GOME-2, a chemical-transport model (with or without assimilation of OMPS limb data) will be needed to represent the stratospheric distributions of these trace gases and enable assignment of slant-column information to the troposphere. A ground pixel size smaller than that of GOME-2 or OMPS, to allow more frequent sounding of the lower troposphere between clouds, would be desirable for future monitoring applications and for AQ forecasting The operational system will provide uv/vis observations at only two local times (9:30am for GOME-2 and 13:30 for OMPS). For AQ forecasting, observations at additional local times would be desirable for trace gas pollutants with short photochemical lifetimes. Similarly for volcanic emission of SO_2. MetOp and NPOESS FTIR sensors will observe several trace gases in addition to H_2O and O_3, principally CH_4 and CO. Height-assignment and height-resolution of these types of observation is intrinsically limited, so they will best be exploited through assimilation. For trace gases other than H2O, sensitivity of the FTIR technique is lowest in the boundary-layer, where temperature contrast with the surface is lowest. Because the MetOp/NPOESS system will have FTIR sensors operating concurrently in at least two different orbits, such observations will be made at four local times per day (equator crossing times: 1:30, 9:30, 13:30 and 21:30). Given the comparatively long photochemical lifetimes of CH_4 and CO, this temporal sampling should be sufficient for most applications. The FTIR spectrometers on MetOp, NPOESS and GOSAT and the near-IR grating spectrometer on OCO will also observe CO_2. Because CO_2 is close to being a uniformly-mixed gas in the troposphere, extremely stringent observational requirements would need to be imposed to quantify perturbations in CO_2 mixing ratio at the amplitudes and spatial and temporal scales required for future monitoring applications. For future research on biogenic emission and uptake of trace gases such as CO_2, CH_4, and N_2O, there will be a demand for remote-sensing measurements on a very fine spatial scale (10's m). This is not attainable from satellite but might be attainable from an aircraft or balloon.

3.4.2 Limitations of Satellite Systems

A number of limitations of the currently planned suite of missions can be identified. In the context of this study these include :

1. Absence of UV/VIS and IR solar occultation for monitoring of stratospheric trace gas and aerosol profiles beyond MAESTRO and ACE on SCISAT, which are unlikely to still be functioning beyond 2010.
2. Requirements for sounding tropospheric trace gases will be addressed by MetOp/NPOESS. To comply better with quantitative requirements, the following would be desirable:
    a. Nadir Thermal IR: spectral resolution similar to TES, i.e. higher than that of CrIS or IASI, to target additional tropospheric trace gases (e.g. NMHCs)
    b. Nadir UV/VIS: observations later in the day than GOME-2 (equator crossing time 9:30am) and OMPS (equator crossing time 1:30pm) for early morning air quality forecast and for detection of afternoon pollution episodes; ground-pixel size smaller than OMPS (50km×50km) to observe the boundary layer more frequently in between clouds, spectral coverage and resolution comparable to GOME-2 (to achieve photometric precision on e.g. NO_2).
3. Requirements for sounding tropospheric aerosol will be addressed by MetOp / NPOESS. To comply better with quantitative requirements, height-resolution would also be desirable, for which spectral coverage of GOME-2 and OMPS does not extend far enough into near-IR. This will be provided by the CALIPSO, ADM-Aeolus and EarthCARE lidars, although only along sub-satellite tracks and only for limited time periods (dictated by laser lifetimes and low orbit heights).
4. Requirements for sounding trace gases and aerosol in the UTLS will not be addressed by MetOP / NPOESS, with the exception of stratospheric O (GOME-2 & OMPS) and aerosol (OMPS). They are at present being addressed by the Odin, Envisat and Aura limb-sounders, but none of these are likely to still be functioning beyond 2010.

Based on the assessment carried out here, Table 3.1 summarises the MetOp/NPOESS non-compliances with respect to the data requirements.

Application	User category		Degree of Metop/NPOESS non-compliance	Notes
Ozone/UV	Protocol	A1S		
	Operational	A2S	Absence of stratospheric data	1
	Assessment	A3S	Absence of stratospheric data	1
Pollution monitoring and AQ forecast	Protocol	B1S	Serious non-compliances on vertical resolution, horizontal & temporal sampling of troposphere	2,3
	Operational	B2S	Absence of data after 1:30pm; serious non-compliances on vertical resolution & horizontal sampling of troposphere	3,4
	Assesment	B3S	Absence of data after 1:30pm; serious non-compliances on vertical resolution & horizontal sampling of troposphere	3,5
Climate	Protocol	C1S	Lack of boundary layer sensitivity for CO, CH_4 & CO_2 and aerosol sensitivity in mid-stratosphere	
	Operational	C2S	Absence of profile data in upper troposphere & stratosphere	5
	Assessment	C3S	Absence of profile data in upper troposphere & stratosphere	5

Degree of MetOp/NPOESS non-compliance:	major	significant	none

Table 3.1 MetOp/NPOESS non-compliance summary table. Degree of non-compliance: **Major** = Key measurements will not be made by MetOp/NPOESS in required height-range and/or time of day; **Significant** = Key measurements made by MetOp/NPOESS will seriously non-comply in vertical resolution, horizontal and/or temporal sampling or precision. Notes:

1. *The only stratospheric data to be supplied by MetOp/NPOESS will be that from OMPS-limb on O_3 and possibly aerosol and NO_2. (Assimilation of data from this type of instrument has not yet been demonstrated by ECMWF or other operational centres.)*
2. *Absence of data later than the 1:30pm OMPS measurement will compromise detection and attribution of pollution episodes occurring in the afternoon and so impact on monitoring of adherence to conventions on long-range transport of air pollution.*
3. *Resolution of height-integrated measurements into atmospheric layers (PBL/free troposphere/stratosphere) wholly dependent on assimilation model vertical structure functions for virtually all constituents.*
4. *Absence of data later than the 1:30pm OMPS measurement will compromise the detection of pollution episodes occurring in the afternoon so impact on the early morning AQ forecast*
5. *Data from ADM-Aeolus or EarthCARE lidar could mitigate MetOp/NPOESS non-compliance on aerosol profile in the troposphere, but assimilation yet to be demonstrated.*

3.4.3 Ground-based Networks

The ground-based networks provide measurements of many of the required products and uncertainty and time-sampling/revisit requirements are met in most cases. The capabilities of these networks is likely to continue to play an important part in monitoring the atmosphere.

It is, however, clear from the assessment that there is, in general, a lack of altitude attribution and that some height ranges are not well addressed. In many cases only surface and column measurements are provided, although height resolved profiles are also specified in the requirements. It should be noted that aerosols, particulates, tracers and some organic compounds are not appropriately addressed for several applications

3.4.4 Conclusion

A comprehensive and objective survey of existing and planned instrument capabilities has been carried out. A large amount of information on instrument performance for current measurement techniques has been collected and assessed in a quantitative manner as far as is feasible. The suitability of existing instrument technology depends on a number of factors including :

- Theme and application to be addressed
- Scope of the satellite mission, including restriction on number of platform, orbits, number and types of sensors and systems
- Importance and priority of particular observations i.e. what is the effect of not achieving particular observational requirements

It is evident from the survey carried out that, while many measurements are made and applications are addressed to various extents, there is scope for improving current techniques and bringing new types of sensor and observation to the available complement of instruments.

In order to define future satellite missions, the potential performance of integrated observing systems, which include satellite and ground-based measurements, and a number of analysis tools, such as specialised retrieval schemes and assimilation systems, must be assessed. The relative timescale of the planned future missions and a potential "Sentinel" is also important so that complementarity can be assured and relevant synergies exploited.

These issues will be addressed in work following this assessment.

4 Identification of new satellite components for integration into the operational observing system

4.1 Introduction – Aims and Objectives

The objective of this work package within the CAPACITY study is to

- Identify the requirements for integrated observing system focussed on Earthwatch target applications

The aims of this work package within the CAPACITY study are

- To provide a vision of integrated observing systems for Earthwatch,
- To identify ground-based, airborne and space-based components to the system that would add value (information) to observables directly required/measured by existing/potential new systems,
- To consider the most pressing application questions and make recommendations as to potential elements of appropriate observing systems.

The report is ordered in terms of a system assessment for each of the selected application areas within the study, namely

a) Stratospheric Ozone and surface UV (§4.2.1)
b) Air Quality (§4.2.2)
c) Climate (§4.2.3)

The data requirements have been taken from the analysis in Chapter 2, based on the analysis of user requirements in Chapter 1, and the quantitative assessment of instrument capabilities *vs* requirements was performed in Chapter 3. In Chapter3, the assessment delivers an appraisal of the missions which currently exist, which exist in the future or which are planned to operate, in particular beyond 2008. However, although the instruments analysed are specific designs, they can be thought of as being representative of that class of instrument e.g. SCIAMACHY, ultra-violet/visible, nadir class, and much of the broader analysis in this work package points towards these broader instrument classes; inherently this identification also points towards instrument heritage which is an important factor in advancing instruments from research to operational missions.

An important aspect of the work reported here is the use of hierarchical diagrams to reflect the variety of instrument types that can contribute aspects of the required information for atmospheric operational services. These diagrams display a "hierarchy of capability" approach illustrating how designs of mission systems could improve in performance from minimum specification to maximum specification. Departures from the diagonal line shown on each diagram indicate qualitatively the extent to which the instrument type identified is not fully compliant with the user requirements. Thresholds for "significant Capacity capability" for operational missions are identified as well as priority instrument performances. In order to satisfy Capacity requirements for a particular mission concept, missions should have sufficient specification to meet both the threshold requirements and to address the priority instrument performances.

4.2 System Assessment

4.2.1 Stratospheric Ozone and UV

Stratospheric ozone and surface ultra-violet (UV) radiation has been of concern for research investigations and analysis of long term trends since the 1970s. The elements of the observing system concerned directly with stratospheric ozone, although more complicated in terms of the range of atmospheric constituents required, are more mature than those of the corresponding U/V system. The differences lie partly in the more highly variable nature of the factors that control U/V radiation compared to those that are important for ozone. It is also true that integration of relevant observations is more demanding for U/V radiation than for ozone and much work remains to be performed in this area. Since U/V radiation depends fundamentally on knowledge of ozone, principally total column ozone, the ozone system is considered first followed by the equivalent exercise for U/V radiation.

System Overview

The stratospheric ozone system can be divided into four components:

1. Monitoring of total ozone column and ozone profiles
2. Monitoring of emissions of ozone depleting substances, their distributions in the stratosphere and the total chlorine loading of the stratosphere
3. Measurement of parameters which are markers for severe polar ozone loss.
4. Measurement of variables that that are significant for our understanding of ozone changes due to chemistry or changes in dynamical circulation.

Systems are likely to employ a combination of ground-based *in situ* and remote sensing instruments, ozonesondes, and satellites. Aircraft instrumentation, deployed on regular commercial flights, has also made and could continue to deliver a useful contribution.

Current and Planned Missions

In this section, we discuss the implications of the analyses of Chapter 3 for operational monitoring systems that might operate in the future. We concentrate on the space segments of the system.

A1S

A1S requires measurement of ozone columns and ancillary parameters for the determination of ultra-violet radiation at the surface. A number of instrument types fulfil the requirements for ozone columns, most of which are **nadir-viewing UV/VIS** instruments e.g. OMPS, or GOME-2 (which only partially meets the horizontal resolution requirement). **MIR** instruments such as TES may also be utilised. **Nadir-viewing UV/VIS** instruments SCIAMACHY and GOME-2, however, are required to provide solar irradiance and aerosol products appropriate to ultra-violet radiation.

The space component for A1 is well covered by the existing Metop mission providing a heritage of UV-visible measurements of total ozone through GOME-2. In addition, the IASI instrument could provide total ozone column information as a back-up although a quantitative link to the historical ozone record would have to be made; it is interesting to note that ATOVS ozone columns now agree very well on with TOMS and GOME in the tropics (a weekly averaged basis). GOME-2 delivers necessary information for surface UV applications including UV spectral solar irradiance, UV aerosol optical depth and UV aerosol absorption optical depth.

The aerosol parameters from GOME-2 meet the threshold requirements for protocol monitoring but there would be an advantage to the deployment of a new UV-visible instrument with better spatial resolution (<? km) for the aerosol.

A2S

The requirements for near real-time ozone information build on the essential components required to satisfy A1, protocol monitoring, by adding specifications for vertical resolution of ozone (<2 km). In addition, it is desirable but not mandatory to perform measurements for a number of trace gases and particles which control ozone chemistry.

The requirement for ozone profiles with information in the upper troposphere suggests a limb mid-infrared or microwave instrument; UV-visible instruments do not provide good information in the upper troposphere (UT) but do provide good information in the lower stratosphere (LS) and above.

A **limb mid-infrared (MIR)** instrument can deliver information on a large number of species. Amongst its key measurements for NRT are the ability to observe PSC occurrence, HNO_3, enhanced

ClO in the LS and MS, and tracers such as CH_4 and N_2O; SF_6 is also measured although not with the required uncertainty. Hence existing limb MIR instruments can deliver both information on heterogeneous processes and on tracers for transport characterisation. In terms of instrumentation, both existing limb MIR Fourier transform spectrometers, such as MIPAS, and radiometers, such as HIRDLS, can meet the majority of the threshold and many of the target requirements; we assume here that operational products for MIPAS can reach close to required vertical resolutions of 3 km without substantial degradation in performance (uncertainty). However, only radiometers of the HIRDLS-type currently achieve required vertical resolution and horizontal resolution for all species. Hence to meet all requirements, a modification to a MIPAS-type instrument is required for it to achieve 2 km vertical resolution and better horizontal coverage; uncertainty performance would need to be maintained.

Microwave instruments appear best suited to provide a broad range of complementary species (ClO, HCl and N_2O measurements are particularly useful). The unique attributes of microwave measurements are the ability to deliver information in the presence of clouds (e.g. polar stratospheric clouds) and to observe O_3, H_2O, N_2O, HNO_3 and HCl. The MIR instruments can measure these species, except for HCl and not in the presence of the thickest PSCs; the latter probably does not matter for NRT purposes since it is the detection of PSCs and subsequent denitrification that matters. Therefore the key aspect for use of existing microwave instruments lies in the potential ability to detect HCl.

Aerosol absorption optical depths are an important measurement for NRT applications and could be met by SAGE III, for example. However, it is also the case that infra-red occultation and infra-red emission measurements could provide information although extinction measurements would not be sensitive to post-Pinatubo “background” aerosol.
From remaining measurements, it is likely that the chief issue remaining is the measurement of LS NO2. A UV-visible instrument would be most suited to this and existing OSIRIS-type observations can provide the required uncertainty, albeit preferably with an improvement in horizontal resolution.

A3S

A3S is very similar to A2S in broad outline. The major difference now is that measurements of trace gases and particles (PSCs) are now essential to deliver a significant Capacity capability.
Metop measurements can only provide a starting point through GOME-2 measurements. IASI measurements of UT H_2O are complementary to GOME-2 data and provide further weight to the planned suite of operational atmospheric observations. However for A3S, a limb instrument component is clearly missing but there are existing instruments which fulfil many of the requirements.
A limb mid-infrared (MIR) instrument can deliver information on a large number of species. Amongst its key measurements for NRT are the ability to observe PSC occurrence, HNO_3, enhanced ClO in the LS and MS, and tracers such as CH_4 and N_2O; SF_6 is also measured although not with the required uncertainty. Hence existing limb MIR instruments can deliver both information on heterogeneous processes and on tracers for transport characterisation. The **limb-viewing MIR** instrument, HIRDLS, already meets requirements for H_2O, N_2O, CH_4, PSC occurrence, SO_2, CFC-11, CFC-12 and HNO_3, and $ClONO_2$ for part of the height range. TES or MIPAS (also **limb-viewing MIR**) will cover molecules such as SO_2, but improved capabilities are required e.g. 3 km vertical resolution and better than 50% uncertainty for SO_2. Similarly, SCIAMACHY (**limb UV/VIS**) is of use for O_3, NO_2 and BrO, but requires better horizontal and vertical resolution for the latter. Microwave instruments could provide complementary measurements of O_3, ClO (MS), HNO_3, H_2O, tracers, and HCl. Occultation instruments could be more important in A3S than A2S because they might measure stratosphere aerosol, HCl and CO with good precision. Overall, the instrument performances and requirements for A2 and A3 are similar. The chief differences lie in the addition of (H)CFCs and BrO, measured by **mid-MIR** and **UV/VIS** instruments respectively, with some increased attraction to solar occultation instruments. Some improvements in MIR instruments performance may be necessary to achieve uncertainty requirements for CH_3Cl and SO_2 enhanced. It is not clear how HBr and $BrONO_2$ are addressed with existing instrumentation.

A1G

Existing **in-situ** measurements fulfil the majority of the requirements for surface measurements; **FTIR occultation** provides total column O_3, CFC-11, CFC-12, HCFC-22. However, for historical continuity and accuracy, we would expect that **Dobson/Brewer** measurements would continue to be made. Measurements of CFC-113 and CH_3CCl_3 are missing.

A2G

A range of instruments is useful for these measurements; **DIAL**, **UVV DOAS**, **MWAVE radiometer** and **FTIR occultation** all uniquely provide at least one of the measurements.

A3G

Again, a combination of **in-situ**, **MWAVE**, **FTIR** and **UVV DOAS** are all used for the measurements that can be made. Essentially, existing systems for A1 and A2 meet and can contribute to aspects of A3. Vertical resolution is desirable – balloon and aircraft measurements may be suitable techniques to cross the gap.

System Concept

An outline system concept for stratospheric ozone and U/V radiation is given in Figure 2.1.1. It consists of the following key elements as linkages.

a) Ground-based measurements for O_3 and (H)CFCs for trends in ozone and chlorine loading (largely based on the Network for Detection of Stratospheric Change).
b) Existing satellite observations supplemented by a suggested annual balloon programme for total chlorine (Cl_y) and total nitrogen (NO_y).
c) Dedicated satellite observation
d) An assessment system and U/V monitoring/forecast system incorporating both direct analysis of the observations, e.g. for trends, and data assimilation systems.

The analysis here largely concentrates on the space-borne component of the required systems. Analysis of the input information shows clearly that there is an increasing system complexity from A1 to A3. MetOP and NPOESS will provide a backbone for these systems but dedicated measurements are also necessary for A2 and A3 in particular. Figure 2.1.1 illustrates the broad concept of these systems.

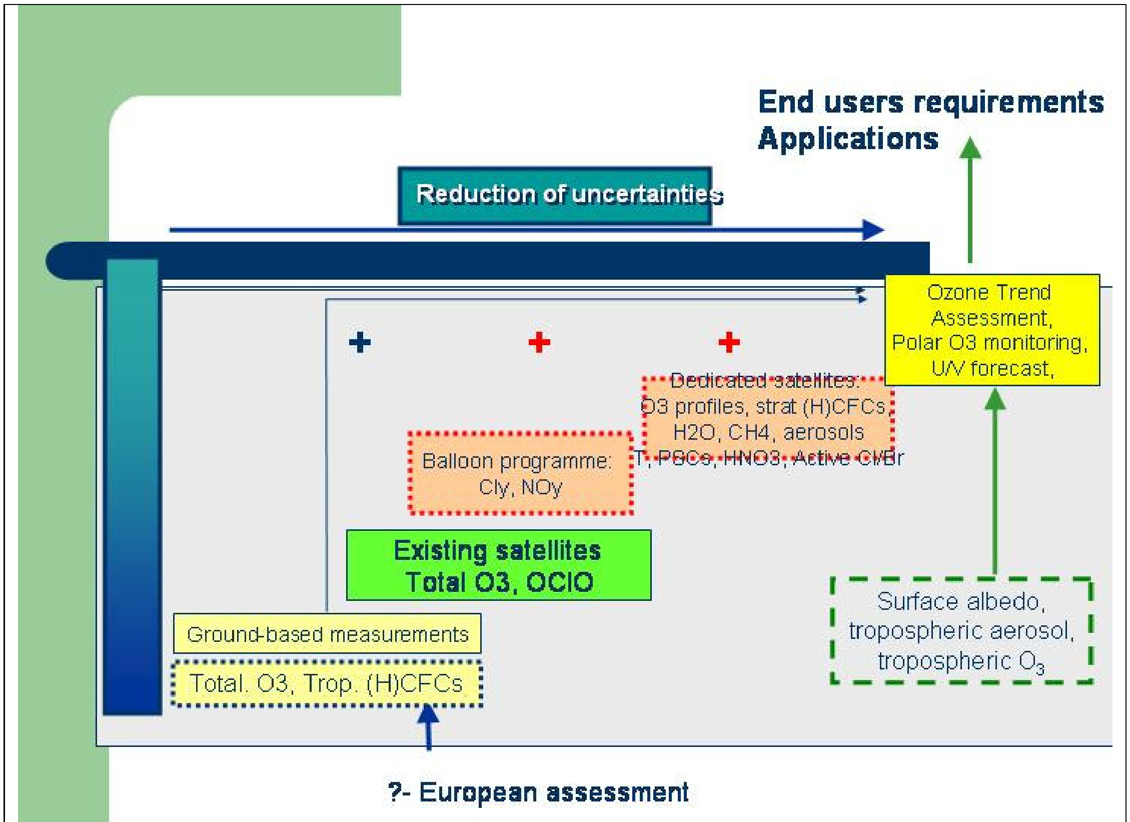

Figure 4.2.1.1 – System concept for UV/Ozone monitoring system

The following analysis and diagrams describe space system concepts for the three cases A1S-A3S. On each diagram we indicate how each advance in instrumentation improves the performance of the system from one that meets the minimum specification to concepts that could potentially meet the full specification. We also make recommendations for study of new instrument concepts.

A1S

Mission concept:

- Metop (GOME-2), ideally with new nadir UV aerosol instrument at high spatial resolution
- Re-visit time and global coverage suggests LEO implementation if a new nadir instrument is implemented.

Recommendations for Mission Concepts:

- New nadir UV aerosol instrument with 10 km horizontal spatial resolution should be studied but with low priority.
- Further information on measurement of UV surface albedo would be good.

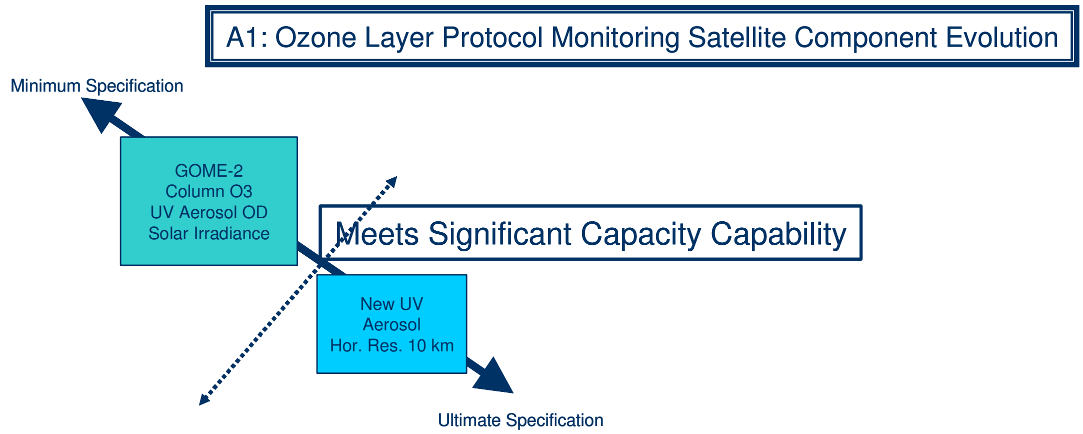

Figure 4.2.1.2 – A1 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

A2S

Mission concept:

- We assume the operation of Metop (GOME-2 and IASI).
- A new MIR limb emission instrument (2 km vertical resolution) is desirable to measure standard species, particularly O_3, and ClO (LS) and PSC detection.
- A microwave limb for instrument for standard species, particularly O_3, and ClO (MS) and HCl is complementary or an alternative.
- A solar occultation instrument, such as SAGE II, is required or else aerosol surface area should be measured by one of the other limb instruments.
- Add limb UV-vis for NO_2 (or potentially for aerosol)
- Add new nadir UV aerosol OD
- Re-visit time and global coverage suggests LEO implementation

Recommendation for WP3000:

- Priority 1 is a limb instrument to measure O3 profiles at the required vertical resolution and, if possible, to obtain additional species.
- A new i/r limb emission instrument with sufficient uncertainty performance to MIPAS but 2 km field-of-view should be investigated. Species are: O_3, ClO (LS), HNO_3, H_2O, tracers, PSCs. The ClO and PSCs probably dictates an FTIR system such as MIPAS.
- New microwave is an alternative to the MIR instrument but is more likely to be targetted towards ClO (MS) and HCl to provide complementary measurements.
- Priority 2 is to fly either SAGE or to determine surface area from MIR or UV-vis limb.
- New UV-VIS NO_2 instrument or SCIA NO_2 limb (reduced performance) would be a useful add-on.
- New UV aerosol nadir instrument (10 km horiz. Resn.) would be useful but low priority.

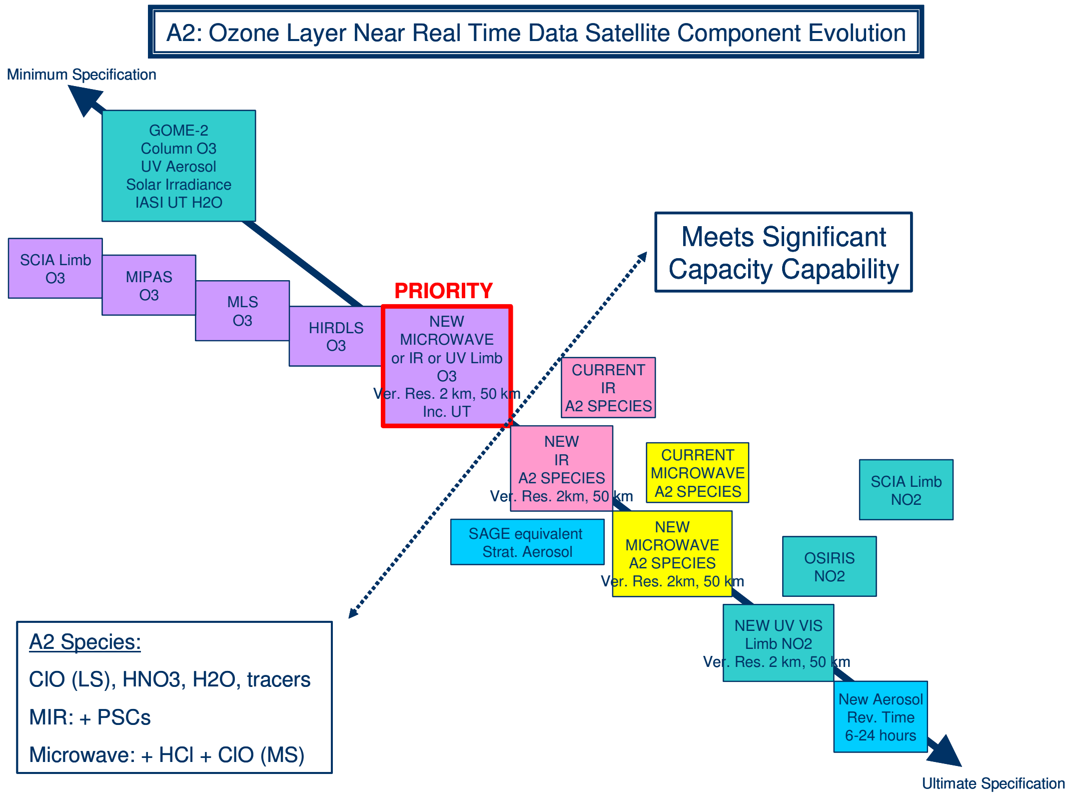

Figure 4.2.1.3 – A2 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

A3S

Mission concept:

- Metop (GOME-2 and IASI)
- Add SAGE or include aerosol surface area in one of the limb instruments below.
- Add infra-red instrument: either MIPAS or a new instrument with preferably 2 km vertical resolution. It should measure standard species plus ClO (LS), PSCs, (H)CFCs, ClONO2.
- As a complementary measurement or as an alternative, elements of existing microwave (SMR type) or a new instrument with preferably 2 km vertical resolution could be implemented for standard species and ClO (MS), SO2 (enh.) and HCl.
- Add limb UV-vis for NO2 and BrO.
- Add new UV-nadir for aerosol OD
- Re-visit time and global coverage suggests LEO implementation

Recommendation for Mission Concepts:

- Priority 1 is to choose to fly either SAGE or to determine surface area from i/r or UV-vis.
- Priority 2 is consider whether new i/r with at least similar uncertainty performance to MIPAS but 2 km field-of-view for O_3 is cost-effective. Species are: O_3, ClO (LS), HNO_3, H_2O, (H)CFCs, tracers, PSCs. Measurements of ClO, PSCs, HCFC-22 probably dictate an FTIR system such as MIPAS.
- New microwave with 2 km vert resn. is an alternative to IR instrument but is more likely to be targetted towards ClO (MS) and HCl to provide complementary measurements.
- A new UV-VIS NO_2 and BrO instrument or SCIA NO_2 and BrO limb (reduced performance) would be a useful add-on.
- New UV aerosol nadir instrument (10 km horiz. resn.) would useful but low priority.

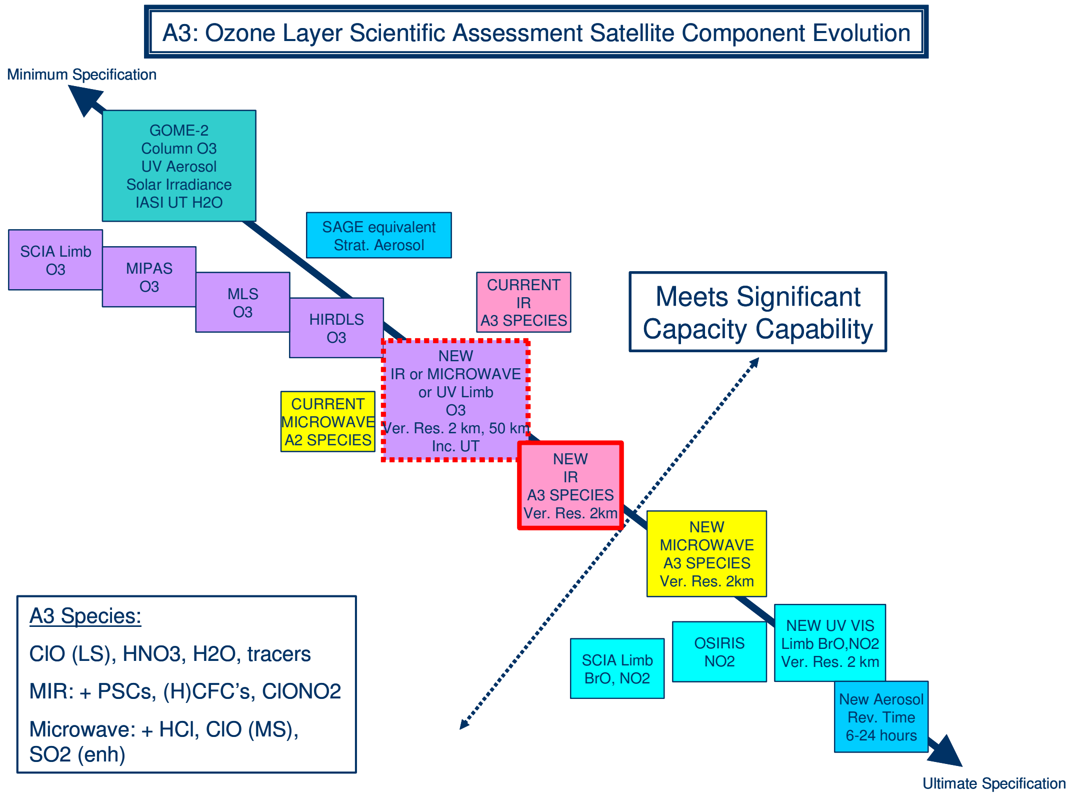

Figure 4.2.1.4 – A3 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

Future Requirements
Table 4.2.1.1 lists the consolidated requirements for ozone/UV satellite measurements. The table is colour coded to reflect how well current/planned systems meet the requirements. The order of table reflects the importance of the measurement to the achievement of the system.

Table 4.2.1.1 - Consolidated requirements for ozone satellite measurements (data merge of all satellite requirements from WP2100)

Requirement / Data Product	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	UT	20 / 100	05 / 2	6 / 24*3	20%
	LS	50 / 100	0.5 / 2	6 / 24*3	20 [10] %
	MS	100 / 200	2 / 3	6 / 24*3	20%
	US+M	100 / 200	3 / 5	12 / 24*7	20%
	Troph column	10 / 50	--	6 / 24*3	20%
	Total column	50 / 100	--	24 ([6]) / 24*3	3 [10] %
Spectral UV surface albedo	Surface	10 / 50	--	24 ([6]) / 24*3	0.1
Spectral UV solar irradiance	TOA	--	--	Daily / Monthly	25 ([2]) %
UV AOD	Total column	10 / 50	--	24 ([6]) / 24*3	0.1
UV aerosol absorption OD	Total column	10 / 50	--	24 ([6]) / 24*3	0.02
Strat AOD	LS	50 / 100	0.5 / 2	6 / 24*3	0.05
	MS	50 / 200	1 / 3	12 / 24*7	0.05
	Stratosphere	50 / 200	--	6 / 24*7	0.05
ClO	LS	50 / 200 [100]	2 [1] / part. column [3]	24 [1]2 / 24*7 [24*3]	50 [30] %
	MS	100 / 200	2 / part. column [3]	24 [12] / 24*7	50 [30] %
	Stratosphere	50 / 200	--	24[12] / 24*7	50 [30] %
NO_2	LS	50 / 200 [100]	2 [1] / part. column [3]	24 [12] / 24*7 [24*3]	20 [30] %
	MS	100 / 200	2 / part column [3] --	24 [12] / 24*7	20 [30] %
	Stratosphere	50 / 200		24 [12] / 24*7	20 [30] %
PSC occurrence	LS	50 / 100	0.5 [1] / 2 [3]	6 [12] / 24*3	<10% mis-assignments
SF_6	LS	50 / 200	1 / 2	6 / 24*3	10%
	MS	100 / 200	2 / 3	12 / 24*7	10%
CO_2	LS	50 / 200	1 / 2	6 / 24*3	10%
	MS	100 / 200	2 / 3	12 / 24*7	10%
H_2O	UT	20 / 100	0.5 / 2	6 / 24*3	20%
	LS	50 / 100	1 / 2 [3]	6 [12]/ 24*3	20 [15] %
	MS	100 / 200	2 / 3	12 / 24*7	20 [15] %
	US	100 / 200	3 / 5	12 / 24*7	15%
	Stratosphere	50 / 200	--	12 / 24*7	15%
N_2O	LS	50 / 100	1 / 2 [3]	6 [12] / 24*3	20 [10] %
	MS	50 [100] / 200	2 / 3	12 / 24*7	20 [10] %
	US	50 [100] / 200	3 / 5	12 / 12 / 24*724*7	20 [10] %
	Stratosphere	50 / 200	--		10%
CH_4	LS	50 / 200	1 / 2 [3]	6 / 24*3	20 [10] %
	MS	100 / 200	2 / 3	12 / 24*7	20 [10] %
	US	100 / 200	3 / 5	12 / 24*7	10%
	Stratosphere	50 / 200	--	12 / 24*7	10%
HCl	LS	Co-located with O_3 [50 / 100]	Co-located with O_3 [1 / 3]	Co-located with O_3 [12 / 24*3]	20 [30] %
	MS	100 / 200	2 / 3	12 / 24*7	30%
	Stratosphere	50 / 200	--	12 / 24*7	30%
HNO_3	LS	Co-located with O_3 [50 / 100]	Co-located with O_3 [1 / 3]	Co-located with O_3 [12 / 24*3]	20 [30] %
	MS	100 / 200	2 / 3	12 / 24*7	30%
	Stratosphere	50 / 200	--	12 / 24*7	30%
CO	UT+LS	Co-located with O_3	Co-located with O_3	Co-located with O_3	20%
CFC-11	LS	50 / 100	1 / 3	12 / 24*3	5%
	MS	100 / 200	2 / 3	12 / 24*7	5%
	Stratosphere	50 / 200	--	12 / 24*7	5%
CFC-12	LS	50 / 100	1 / 3	12 / 24*3	5%
	MS	100 / 200	2 / 3	12 / 24*7	5%
	Stratosphere	50 / 200	--	12 / 24*7	5%
HCFC-22	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	100 / 200	2 / 3	12 / 24*7	20%
	Stratosphere	50 / 200	--	12 / 24*7	20%
BrO	LS	50 / 100	1 / 3	12 / 24*3	30%
	MS	100 / 200	2 / 3	12 / 24*7	30%
	Stratosphere	50 / 200	--	12 / 24*7	30%
Aerosol surface density	LS	50 / 100	1 / 3	12 / 24*3	100%
	MS	100 / 200	2 / 3	12 / 24*7	100%
	Stratosphere	50 / 200	--	12 / 24*7	100%
HBr	LS	50 / 100	1 / 3	12 / 24*3	30%
	MS	100 / 200	2 / 3	12 / 24*7	30%
	Stratosphere	50 / 200	--	12 / 24*7	30%

$BrONO_2$	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	30% 30% 30%
Ch_3Cl	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	30% 30% 30%
Ch_3Br	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	30% 30% 30%
SO_2 enhanced	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	5% 5% 5%
Volcanic aerosol	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	50% 50% 50%

(A2S- requirement), [A3S – requirement]

Requirements can be met by current instruments

Some requirements met

No requirements met

In summary, what is required is

- Limb instrument(s) that measures a range of trace species and complements the Nadir measurements made on Metop/NPOESS.
- Implementation options include a limb-MIR, in combination with a limb microwave instrument in order to meet the optimal number of requirements. However, a single instrument of either type would provide significant aspects of the system.
- A limb UV/VIS system to measure NO_2 and potentially BrO would be invaluable.
- Ground-based systems provide a total ozone verification system, validation and source gas monitoring, but cannot provide the range of height resolved information required.

4.2.2 Regional Air Quality

Air quality (AQ), i.e. gaseous pollutants and particulate matter impacts from the urban and regional scale to the global scale. AQ on these scales has implications for a number of contemporary issues including:

- Human health, (e.g. respiratory, cancer, allergies…),
- Eco systems (e.g. crop yields, acidification / eutrophication of natural ecosystems),
- National heritage (e.g. buildings),
- Regional climate (aerosol and ozone exhibit a strong regionality in climate forcing).

Primary pollutants (*e.g.* CO, SO_2, NO_2 and volatile organic compounds (VOCs) - The primary pollutants are those directly emitted into the atmosphere from a range of anthropogenic sources, such as transportation, industrial processes and agriculture. Some VOCs and NO_x have concomitant biogenic sources.

Oxidants -Owing to its toxicity for plants, animals and humans, and its importance as a green house gas, strategies were developed in the US and later in Europe to reduce the levels of ozone in the troposphere both during photochemical episodes and in general. These strategies are not as straightforward as for primary pollutants because ozone is not emitted into the atmosphere but is formed *in situ* from a complex mixture of precursor pollutants (CO, VOCs and NO_x) under the action of ultra-violet radiation from the sun. Therefore ozone abatement strategies must be directed towards lowering the emissions of ozone precursors, NO_x and VOCs. The non-linear influence of NO_x and VOC emissions on ozone formation and destruction, the influence of transport and dispersion processes on the atmospheric distribution of chemical compounds, and the vast differences in their chemical lifetimes require thorough scientific understanding for the design of successful abatement strategies.

Aerosol – Aerosols affect life on earth in several ways. They play an important role in the climate system; the effect of aerosols on the global climate system is one of the major uncertainties of present climate predictions. They play a major role in atmospheric chemistry and hence affect the concentrations of other potentially harmful atmospheric constituents, e.g. ozone. They constitute an important controlling factor for the radiation budget, in particular in the UV-B part of the spectrum. At ground level, they can be harmful, even toxic, to man, animals, and plants. Because of the adverse effects that aerosols can have on human life, it is necessary to achieve an advanced understanding of the processes that generate, redistribute, and remove aerosols within the atmosphere.

The user requirements with respect to AQ have been detailed in Chapter 1.

System Overview

In general terms, the system should be able to for key policy relevant gas-phase and particulate species

- Establish pollutant concentrations, deposition, emissions and transboundary fluxes on the regional scale, including intercontinental transport and boundary conditions for urban AQ,
- Identify trends in time,
- Assess the success of international abatement strategies for atmospheric pollutants,
- Improve the understanding of atmospheric chemical and physical processes and provide data for the validation of models,
- Provide data which, in conjunction with models, are the basis for the assessment of environmental problems related to air pollution,
- Provide measurements required to assess the effects of atmospheric pollutants,

- (adapted from EMEP observation strategy).

The likely information requirements for a rationale air quality system are given in Figure 2.1.1. Systems are likely to employ a combination of ground-based *in situ* and remote sensing instruments, sondes, and satellites. Aircraft instrumentation, deployed on regular commercial flights, has also made and could continue to deliver a useful contribution. The current air quality system throughout Europe consists of an expensive non-integrated series of measurements *viz*

1. Background sites
2. Regional master sites
3. Local monitoring networks
4. Aircraft measurements
5. Passenger aircraft
6. Satellite measurements

Current Planned/Missions

B1S

The requirements make clear that instruments should be sensitive to the Planetary Boundary Layer (PBL). Re-visit times of 2 hours are threshold requirements. Horizontal resolutions should ideally be better than 20 km with a target of 5 km. Nighttime measurements would be ideal, as well as daytime measurements. Both trace gas and aerosol information are required

Metop provides a basic set of measurements through GOME-2 (O_3, NO_2, SO_2, HCHO) and IASI (CO). Aerosol information is likely to be available from GOME-2 and AVHRR but with caveats on uncertainty and spatial resolution achieved. Combination of O_3 data from GOME-2 and IASI could provide greater height resolution in the PBL and free troposphere. Development work to support this product is highly recommended.

However, in order to support air quality monitoring, it is quite clear that a new mission is required. For this purpose, a number of instruments measure one or more products. A **Nadir-UV/VIS** instrument such as SCIAMACHY/OMI can measure the largest number of relevant trace gases, for example SO_2 and CH_2O, but only delivers height resolved data for O_3. Others, for example the **nadir-MIR** TES or IASI, are sensitive to the lower layers, but with insufficient vertical resolution compared to that desired.

- Re-flight of an ice-free SCIAMACHY nadir near infra-red instrument could give better information on CO. Similar combination with nadir-MIR could be performed for CO to advantage if a near infra-red instrument could be flown to complement MetOp.
- Re-flight of an existing aerosol instrument could deliver required aerosol information at 550 nm. A new instrument achieving better uncertainty performance is highly desirable.

The key question is how to meet the revisit time requirement (2 hours max, preferably 0.5 hours) while maintaining the high horizontal and vertical resolution. The greatest requirement for the mission is frequent re-visit time (< 2 hours) as well as high spatial resolution (< 20 km). This is not met by existing orbital elements such as MetOp and is necessary to meet existing basic operational modes.

B2S

B2S is very similar to B1 with the addition of vertically resolved H_2O and nitrogen compounds in the PBL; near-surface H_2O is desirable for boundary layer chemistry. For B2S, the other major difference is the fact that HNO_3, N_2O_5 (night) and PAN are desirable nitrogen compound measurements which could significantly enhance near real-time operational air quality services.

As for B1, re-visit time and spatial resolution are the priority improvements to current or planned missions. IASI is close to meeting requirements for near-surface H2O, although other sensors could meet requirements for H2O columns. Improved aerosol instrumentation is desirable. **Nadir-UV/Vis** instruments can provide some of the measurements if suitably enhanced and deployed. The nitrogen species have not been measured from space until now, but, combined with the desirability of nighttime measurements and CO, suggests that **nadir-MIR** should be investigated for future contributions to air quality systems. **Nadir-SWIR** (short wave infra-red) observations can also provide CO. Hence to meet air quality requirements, neither the planned missions nor existing instruments as deployed are satisfactory. Re-visit time is often critical.

B3S

The analysis for B3S is the same as B2S, apart from **organic nitrates**, for which no measurement techniques are currently available. For scientific assessment, multi-spectral AOD and aerosol type arguably become more important. Aerosol multi-spectral AOD and aerosol type are not measured adequately by current or planned missions.

B1G

There are a lot of gaps in the measurements. **In-situ** measurements make a number of the surface measurements; a few other instruments may be used e.g. **O_3 sondes**, but these fail the revisit requirements. Others fail for other reasons e.g. **FTIR** CO measurements do not the required vertical resolution, **DIAL** for O_3 the uncertainty in the PBL.

B2G

In-situ data meets a lot of the surface requirements. **O_3 sondes** are useful, but their revisit time is poor.

B3G

Analysis Few of the requirements are met, less than B2G.
Conclusions As B2G.

System Concept

An outline system concept for air quality is given in Figure 4.2.2.2. It consists of the following key elements as linkages.

a) Ground-based measurements
b) Existing satellite produce observations
c) Dedicated satellite observation
d) A data assimilation system to produce an air quality management and forecast system,

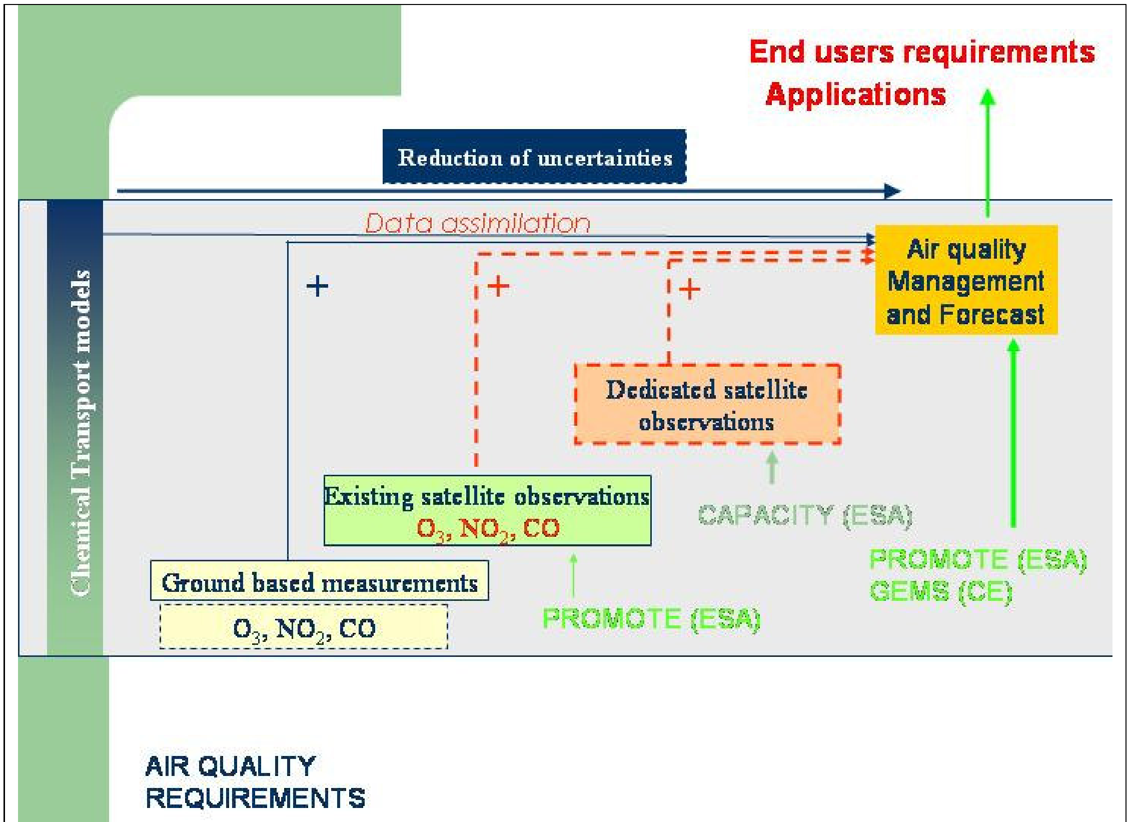

Figure 4.2.2.2 – System concept for AQ

The following sections and diagrams (4.2.2.3-4.2.2.5) describe space system concepts for the three cases. On each diagram we indicate how each advance in instrumentation improves the performance of the system from one that meets the minimum specification to concepts that could potentially meet the full specification. We also make recommendations for study of new instrument concepts.

B1S

Mission concept:

- Frequent re-visit time and high spatial resolution (<20 km)
- Options could be GEO or LEO or a combination of both.
- If LEO, then an enhancement of the Metop/NPOESS systems would be necessary both for complement of species and for coverage/spatial resolutions.
- Species: O_3, NO_2, SO_2, HCHO, CO, aerosol AOD (550 nm), multi-spectral AOD for aerosol size.
- Instruments are likely to be UV-visible (O_3, NO_2, SO_2, HCHO, aerosol) and infra-red or shortwave infra-red for CO. The infra-red can also supply complementary information for O_3.
- There is a requirement for an enhanced aerosol instrument/system delivering uncertainties of < 0.05 in aerosol optical depth at 10 km spatial resolution and enhancing our ability to discriminate aerosol type.
- Limb instruments would enable better correction for upper parts of NO_2, O_3, and CO.

Recommendation for Mission Concept studies:

- Both GEO and LEO options should be studied.
- Priority 1 is to achieve the re-visit time with high spatial resolution as the 2nd priority.
- A key decision concerns our ability to measure CO. Flight of both an infrared and near infrared instrument would provide the greatest performance but would add to mission complexity.

- Multi-spectral aerosol information with improved uncertainty (equivalent to <0.05 nm at 550 nm) would be ideal. Aerosol type measurements are also useful.

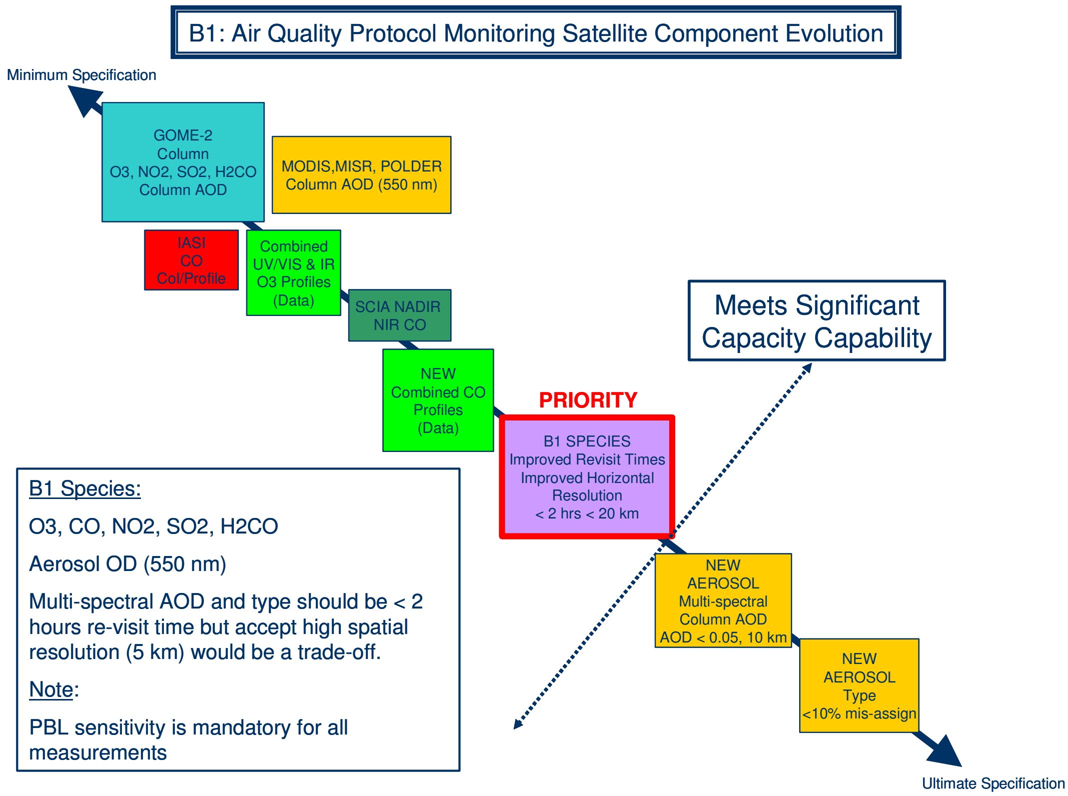

Figure 4.2.2.3 – B1 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

B2S

Mission concept:

- As for B1, GEO or LEO with frequent re-visit time (<2 hours) and high spatial resolution (< 20 km)
- Aerosol instrument with better uncertainty (<0.05 optical depth at 550 nm) at high spatial resolution (10 km).
- System to include measurement of CO.
- LEO could use IASI measurements of H2O. GEO would need to include H2O measurements
- An instrument to measure PAN, HNO_3, N_2O_5 (night) would be ideal. A nadir MIR FTS instrument should be considered for these compounds and for nighttime measurement capability.
- Limb instruments would enable better correction for upper parts of NO_2, O_3, CO and HNO_3 columns.

Recommendations for Mission Concept studies:

- As for B1.
- Instrument to measure H2O from GEO
- Instrument to measure PAN, HNO_3, N_2O_5 - nadir MIR FTS

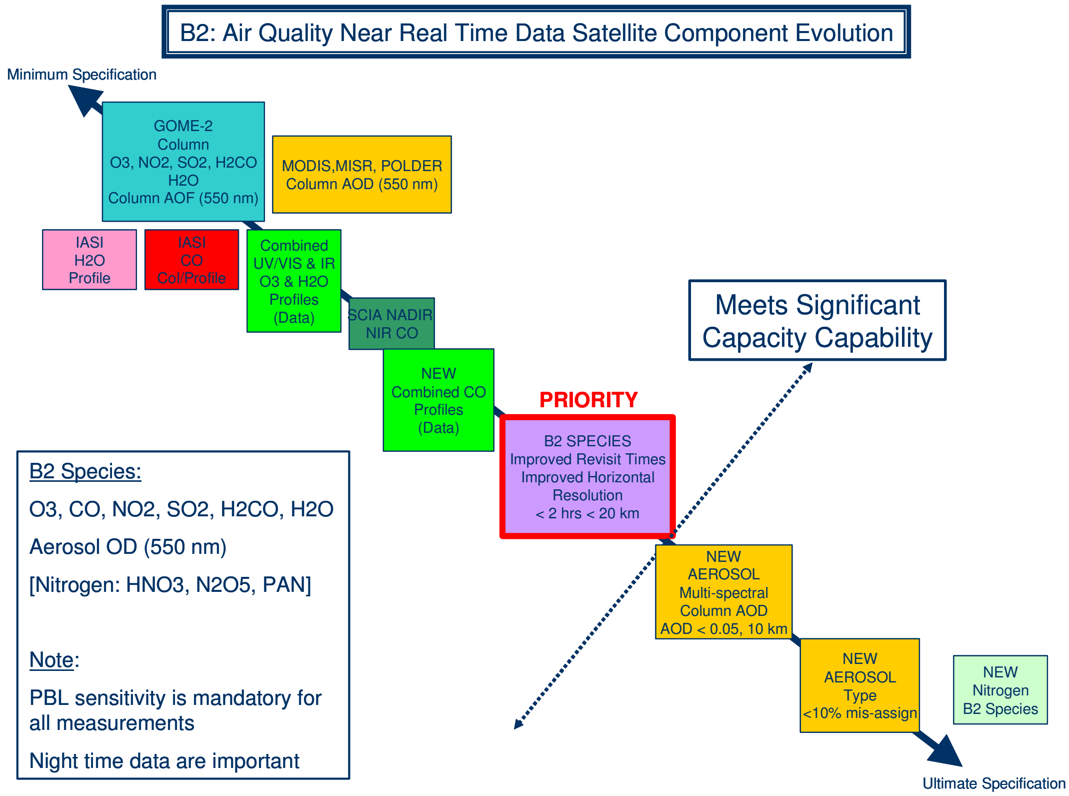

Figure 4.2.2.4 B2 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

B3S

Mission concept:

- As for B2, GEO or LEO with frequent re-visit time (<2 hours) and high spatial resolution (< 20 km)
- Aerosol instrument with better uncertainty (<0.05 optical depth at 550 nm), multi-spectral for aerosol size but also for aerosol type.
- An instrument to measure PAN, HNO_3, N_2O_5 (night) and organic nitrates would be ideal. A nadir MIR FTS instrument should be considered for these compounds and for nighttime measurement capability.
- Limb instruments would enable better correction for upper parts of NO_2, O_3, CO and HNO_3 columns.

Recommendations for Mission Concept studies:

- As for B2.
- Instrument to measure aerosol type as well as multi-spectral for aerosol size.
- Instrument to measure PAN, HNO_3, N_2O_5 and organic nitrates – nadir MIR FTS.

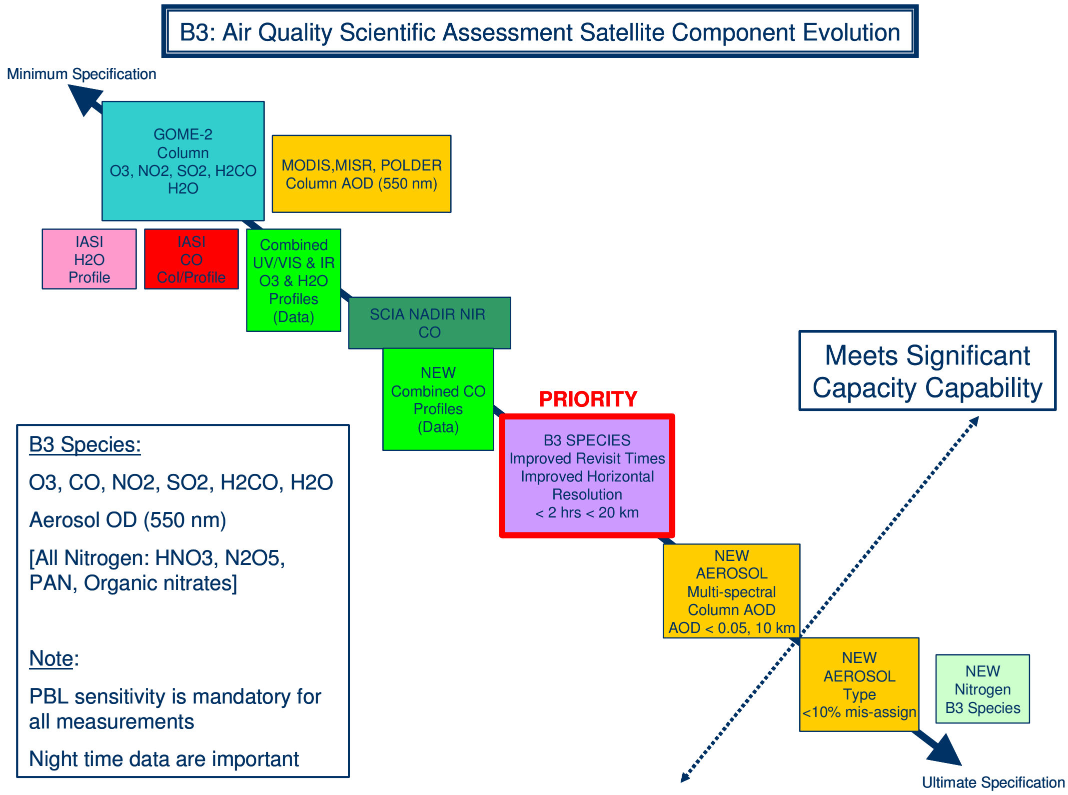

Figure 4.2.2.5 – B3 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

Future Requirements

It is quite clear that only an integrated system of satellite measurements coupled to the appropriate ground-based measurements will be able to fulfil the user requirements for AQ.

Currently low earth orbit satellites present a quasi-synoptic view of regional AQ with revisit times between one and six days. It is clear that, given the rate of change of aerosol and oxidant concentrations in the boundary layer, shorter revisit times are required. One strategic option available is the measurement of tropospheric composition from geostationary orbit. An instrument on a satellite in geostationary orbit would have the ability to make high spatial- and temporal-resolution measurements of atmospheric composition. It is likely as shown in Figure 2.2.2 that the data from satellite must be combined with other sources of data (e.g. aircraft, vertical soundings, and selected ground-based data) that do not require a-priori information from models.

It is clear that high temporal sampling, small spatial resolution measurements of BL atmospheric constituents from space required as part of any rational AQ measurement system. With respect to how may quantify that statement, in order to compliment ground-based measurements spatial resolution should be or the order of 5 km (see WP2100) and the temporal resolution in the order of 0.5 h. Table 4.2.2.1 gives the consolidated requirements for AQ satellite measurements.

Table 4.2.2.1 - Consolidated requirements for AQ satellite measurements (data merge of all satellite requirements from Chapter 2)

Requirement / Data Product	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty	Notes
O_3	PBL FT	5 / 20 5 / 50	-- 1 / 3	0.5 / 2 0.5 / 2	10% 20%	

	Tropospheric Column Total Column	5 / 20 50 [5] / 100 [20]	-- --	0.5 / 2 24 (12) [0.5] / 24*3 [2]	25% 3 (5) %	
NO_2	PBL FT Tropospheric column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	10% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2	
CO	PBL FT Tropospheric column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 25% 25 %	
SO_2	PBL FT Tropospheric column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2	
CH_2O	PBL FT Tropospheric column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2	
Aerosol OD	PBL FT Trop. column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- -- -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	0.05 0.05 0.05 0.05	
Aerosol Type	PBL FT Trop. column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- -- -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	< 10% mis-assignments	
H_2O	PBL FT Tropospheric Column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	10% 20% 10% 10%	
HNO_3	PBL FT Tropospheric Column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2	
N_2O_5 (night)	PBL FT Tropospheric Column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 50% 1.3e15 molec cm-2 1.3e15 molec cm-2	
PAN	PBL FT Tropospheric Column Total column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2	
Organic Nitrates	PBL	5 / 20	--	0.5 / 2	30%	B3S only
Spectral UV surface albedo	Surface	5 / 20	--	24 / 24*3	0.1	

(B2S- requirement), [B3S – requirement]

Requirements can be met by current instruments

Some requirements met

No requirements met

In summary,

- An effective AQ system is going to require a fusion of ground-based and satellite measurements.
- There is a general requirement in AQ for high time resolution measurements, there are a number of potential implementation options
  - Constellation of LEO instruments
  - Instruments in MEO
  - Instruments in Molniya orbit
  - An instrument in a GEO orbit
    - It is recommended to perform a brief trade-off between orbit options.
- With respect to future LEO components the benefits of an additional CO channel in compliment to MetOP should be assessed

- A measurement challenge from space is how to deliver the best height resolved (sensitivity to PBL) information on the target species. A number of implementation options should be explored to look at the best space-borne observing strategy.
  - A combination of UV/VIS and IR (Thermal or Mid) might provide added height information. This synergy should be explored.
- There is requirement for high spatial (horizontal) resolution.
- Need an assessment of aerosol products from space in particular GEO and LEO.
  - User products currently focus on PM size
- It maybe worth looking at a mission envelope that looks at both the minimum and optimal requirements in satellite implementation.
- Any future operational nadir viewing AQ satellite system should explore optimal combination with any limb-type missions.

Beyond the scope of this study there is the requirement for a better assessment of the quantitative benefits of a space-borne system in regional AQ monitoring.

4.2.3 Climate

Within the area of climate there are two different user needs. The first is centred on protocol monitoring and the production of emission databases (C1). The second is centred on using the profile information in the UT/LS as a climate diagnostic (C2+C3).

System Overview

The current climate monitoring system is dominated by ground-based measurement of greenhouse gases that are used for the determination mainly of long-term trends of greenhouse gases. Development work in the current EU project GEMS is using CO_2 satellite data from AIRS.

Current and Planned Missions

The following is an assessment of the ability of current or planned mission to fulfil the user requirements, from the output of WP2200:

C1S

This mission seeks to measure greenhouse gases, CO and aerosols. The mission is intended to be global and have PBL sensitivity for CH_4, CO_2, CO, NO_2. The chief targets are CO_2, CH_4, CO, O_3, NO_2, aerosols. Stratospheric aerosol is required as well as tropospheric aerosols but not with as high a priority.

Metop provides a basis set of measurements with information on CO_2, CH_4 and CO provided by IASI, and O_3 and NO_2 delivered by GOME-2. Existing aerosol instruments can provide useful information although higher accuracy is desirable for tropospheric measurements. Re-flight of an **ice-free SCIAMACHY nadir shortwave infra-red** instrument could give better information on CO_2, CH_4, and CO. Achieving the requirements for CO_2 is very difficult with any current technology suitable for operational implementation and is not strongly emphasized here as a mission driver. Improvements in uncertainty performance for CH_4 would be ideal as well as higher spatial resolution.

Combination of O_3 data from GOME-2 and IASI could provide greater height resolution in the PBL and free troposphere. Development work to support this product is highly recommended. Similar work could be performed for CO with advantage if a near infra-red instrument could be flown to complement Metop.

It is important to note that the analysis implies the mission is similar to B1 but re-visit time not as high a priority (6-12 hours for C1), CH_4 is emphasized for C1 rather than CO. Stratospheric aerosol information desirable for C1 and aerosol type is not as important.

C2S

The mission seeks to derive climate information in near real-time. This mission concept is driven by NRT system assimilation and the improvement in representation of climate from assimilation of observations for rapidly varying constituents. The targets are H_2O (very important), O_3, aerosols/cirrus, stratospheric tracer information. Stratospheric aerosol is required as well as tropospheric aerosols

- IASI on Metop provides a basis set of measurements with vertically resolved information on H_2O and O_3, and column information on CH_4, N_2O and CO_2.
- A set of limb observations are required targetting the UT and stratosphere for H_2O, O_3, UT cirrus and stratospheric tracers.
- Microwave limb measurements which are cloud-free could be most important for H_2O and O3, and there is also useful information on thicker UT cirrus.
- MIR limb instruments tend to provide good tracer measurements. They can also provide measurements of H_2O, O_3 (not in the presence of thick clouds) and also have additional sensitivity to very thin clouds and also to some aerosols.
- Aerosol can be measured adequately in the stratosphere using existing measurements from SAGE. Tropospheric measurements need to meet 0.05 requirement.

- Re-visit time for H_2O is an issue since 6 hours is a threshold and 1 hour is a target. Also for O3 (6 hours target) and aerosol OD (1 hour target).

C3S
The mission seeks to provide a fundamental capability for scientific assessment of the climate system. The mission targets can be sub-divided into radiative forcing, oxidising capacity and stratospheric ozone. There are many target species and domains but the upper troposphere and lower stratosphere (UTLS) are particularly important. We assume that vertical resolution and no. of species is more important than re-visit times.

- Metop provides a starting basis for the measurement system
- A limb MIR FTS instrument meets the major requirement is to provide enhanced capabilities to sound many species in the UTLS in all 3 categories. Its vertical resolution should approach 2 km.
- In addition, the remainder of the ozone system for C3 looks like A3, i.e. with limb MIR, and possibly additional microwave capability, and SAGE aerosol.
- The radiative forcing system for C3 looks like the first part of C2 with tropospheric aerosol required and PBL sensitive CH_4, N_2O as well as Metop.
- The oxidising capacity system for C3 looks like Metop with a MIR limb instrument and possibly UV limb for CH_2O in the UT.

This is a very extensive list of requirements. A lot of these species seem to require a **limb-sounding MIR** instrument; HIRDLS and SCIAMACHY can be used for many of the measurements. MIPAS and TES (**limb-MIR**) are also useful, but fail the vertical resolution requirements for a number of the species. Other instruments, e.g. SMILES and MLS (**limb-MM**) and ACE (**IR occult**) are also needed for some of the measurements.

C1G
For this set of requirements, **in-situ** measurements of the surface often do not have the required uncertainty. **FTIR occultation** makes a number of the column measurements, but again not at the required uncertainty, except for N_2O and CH_4.

C2G
O_3 requirements can be met by **sondes** and **DIAL**, together with another instrument e.g. **FTIR occultation** for the column. The latter is also useful for a number of other measurements, although the vertical resolution needs improving.

C3G
There are a lot of species that are not measured. **In-situ** and **FTIR occultation** might be used for a number of the observations, but uncertainty and vertical resolution are problems.

System Concept

With respect to Protocol monitoring it is clear that the satellite must be able to measure total abundances/global concentrations in terms of monthly means of GHG, the inversion of which can lead to the production of emission products.
The satellite measurements should give dry air mixing ratios with vertical information having significant sensitivity to boundary layer. There are stringent precision target and thresholds for GHG such as CO_2 (3 ppmv threshold, 1ppmv target)
The analysis here largely concentrates on the space-borne component of the required systems. Analysis of the input information shows clearly that there is an increasing system complexity from C1 to C3.
The following analysis and diagrams describe space system concepts for C1, C2 and C3. On each diagram we indicate how each advance in instrumentation improves the performance of the system

from one that meets the minimum specification to concepts that could potentially meet the full specification.

C1S

Mission concept:

- As for B1 with addition of CH_4, stratospheric aerosol and aerosol absorbing OD.
- Metop (GOME-2), ideally with near i/r or mid-infrared nadir instrument and new nadir aerosol instrument at high spatial resolution.
- Re-visit time and global coverage suggests LEO implementation.
- Limb instruments could improve tropospheric data accuracy.

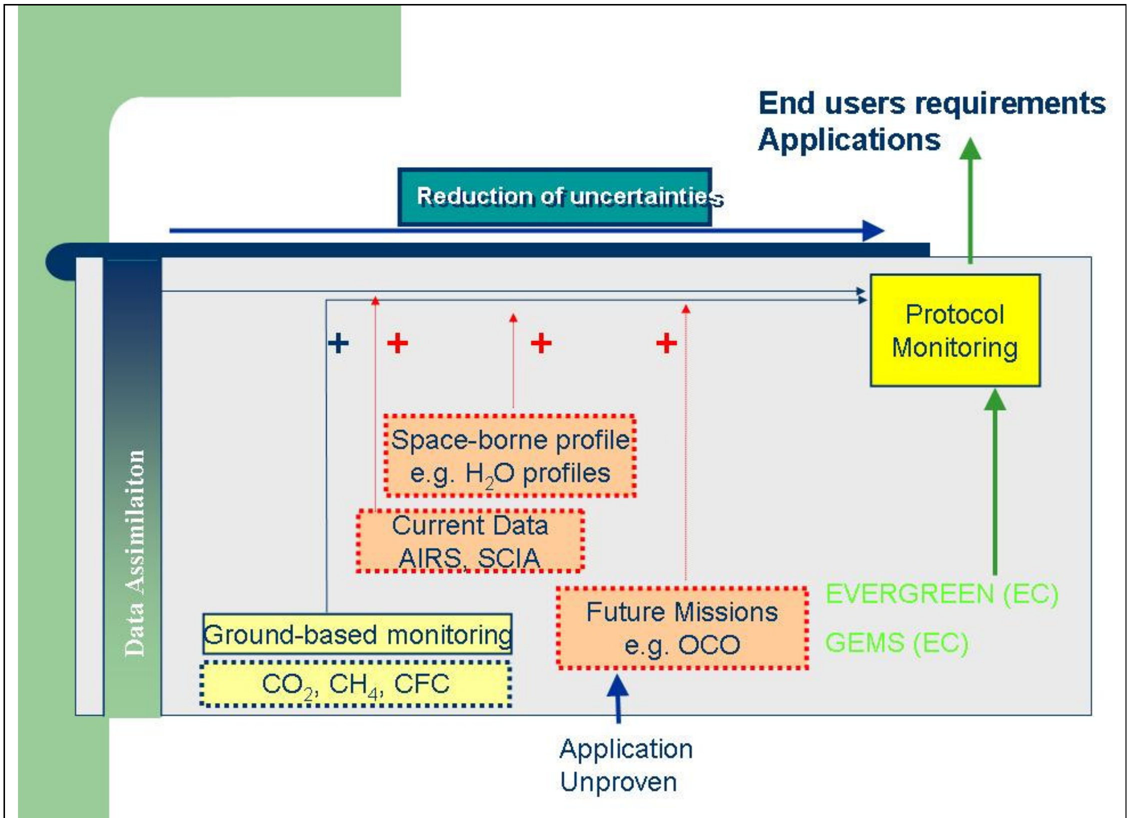

Figure 4.2.3.1 – Outline system concept for Climate monitoring system for protocol monitoring

Recommendations for Mission Concept studies:

- Improved near infra-red instrument should be studied which has high spatial resolution (10 x 10 km) and improved uncertainty for CH_4 (2%).
- New nadir UV aerosol instrument with 10 km horizontal spatial resolution and improved performance for aerosol absorbing AOD (<0.01) should be studied but with low priority. Improved re-visit time could be more important with 6 hours being desirable.
- Stratospheric aerosol instrument should be considered.

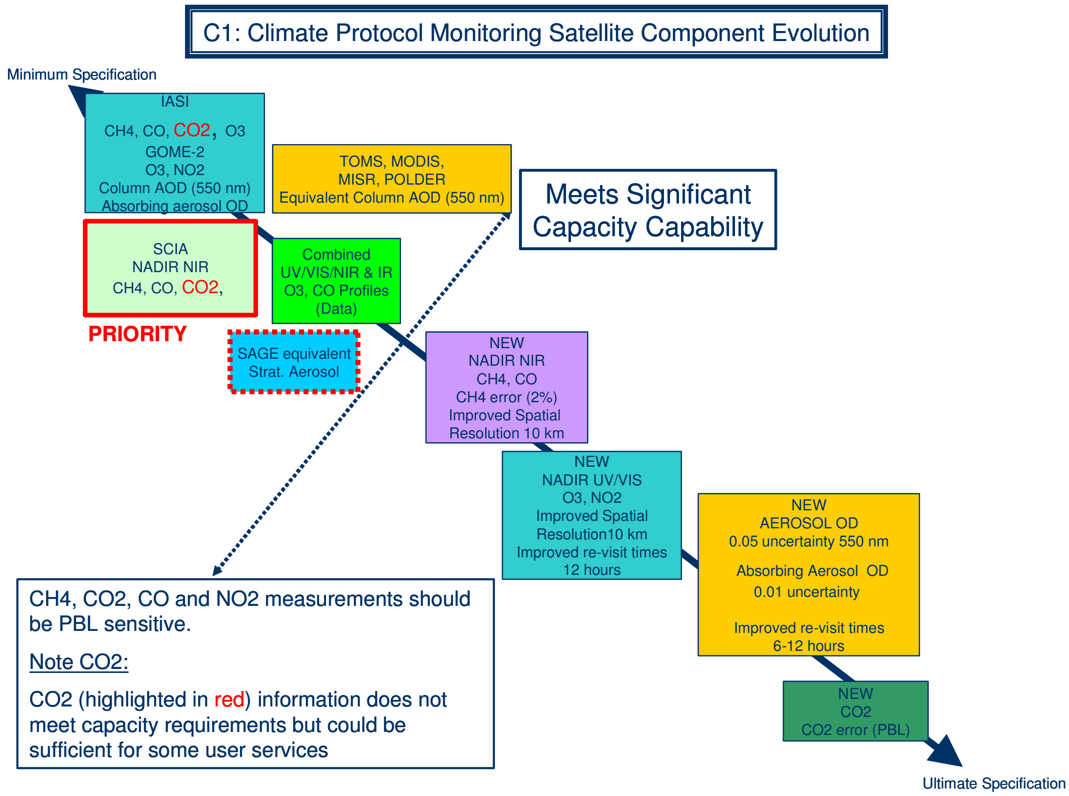

Figure 4.2.3.2 – C1 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

C2S

Mission concept:

- The basic system consists of Metop with a limb system, based around a limb MIR instrument, and a nadir system built around a re-flight of a SCIAMACHY-type nadir system with aerosol capabilities.
- The limb system looks like an MIR FTS (2 km resolution), with additional microwave capability for radiative forcing measurements and HCl/ClO for stratospheric ozone measurements, and possibly a UV instrument for CH_2O UT limb.
- The nadir system consists in part of a LEO system with nadir near i/r and tropospheric aerosol instruments.
- A GEO system would be ideal to meet re-visit time targets for H_2O, O_3, aerosol but would not be global.

Recommendations for Mission Concept studies:

- Examine MIR limb instruments to look ability to achieve wide coverage of species, with 2 km vertical resolution.
- Consider microwave limb instrument concentrating on H_2O, O_3, cirrus OD HCl.
- Also examine a specific limb instrument obtaining information on aerosol.
- Consider an NIR instrument with improvements over SCIAMACHY to deliver ice-free, improved performance for CH_4, CO with higher spatial resolution of 10 km.
- Examine an instrument for tropospheric aerosol which meets uncertainty requirement of 0.05 at spatial resolution of 10 km and can measure absorbing aerosol OD (<0.01).
- Consider how much advantage can be gained from synergies with GEO missions.

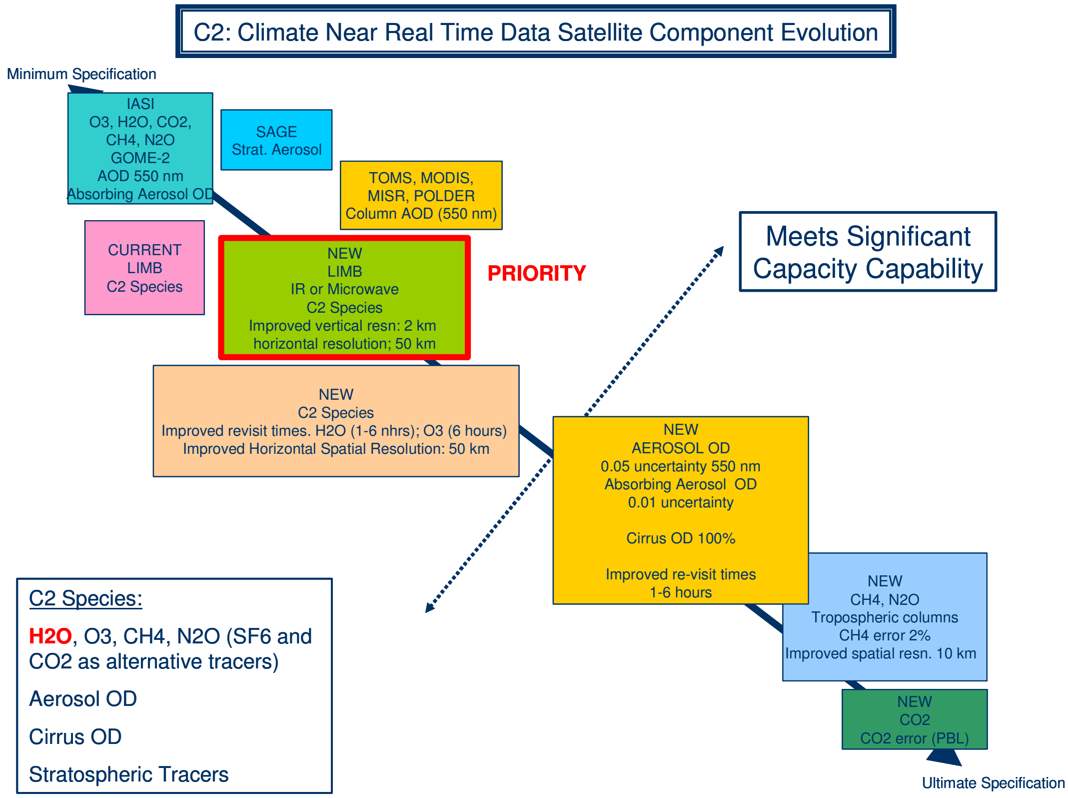

Figure 4.2.3.3 C2 specification diagram. The extremes of this diagram show the ultimate and minimum specification, instrument sets are then transposed onto it.

C3S

Mission concept:

- The mission is quite different from C1 and C2 in terms of issues and species but has instrument elements in common with C2.
- Some information is provided by Metop.
- A limb MIR component is essential to cover the range of species.
- A nadir NIR component and tropospheric aerosol instrument allows radiative forcing issues to be tackled.
- A microwave instrument would be useful to enhance the radiative forcing and stratospheric ozone issues.
- Aerosol information in the stratosphere is required.

Recommendations for Mission Concept studies:

- Examine performance of new limb MIR FTS instrument compared to MIPAS with respect to the full range of species required here.
- Consider an NIR instrument with improvements over SCIAMACHY to deliver ice-free, improved performance for CH_4, CO with higher spatial resolution.
- Examine an aerosol instrument for tropospheric aerosol which meets uncertainty requirement of 0.05 at 10 km spatial resolution and good absorbing aerosol AOD performance.
- Consider how best stratospheric aerosol OD measurements might be performed.
- Consider microwave instrument concentrating on H_2O, O_3, cirrus OD, ClO (MS) and HCl.

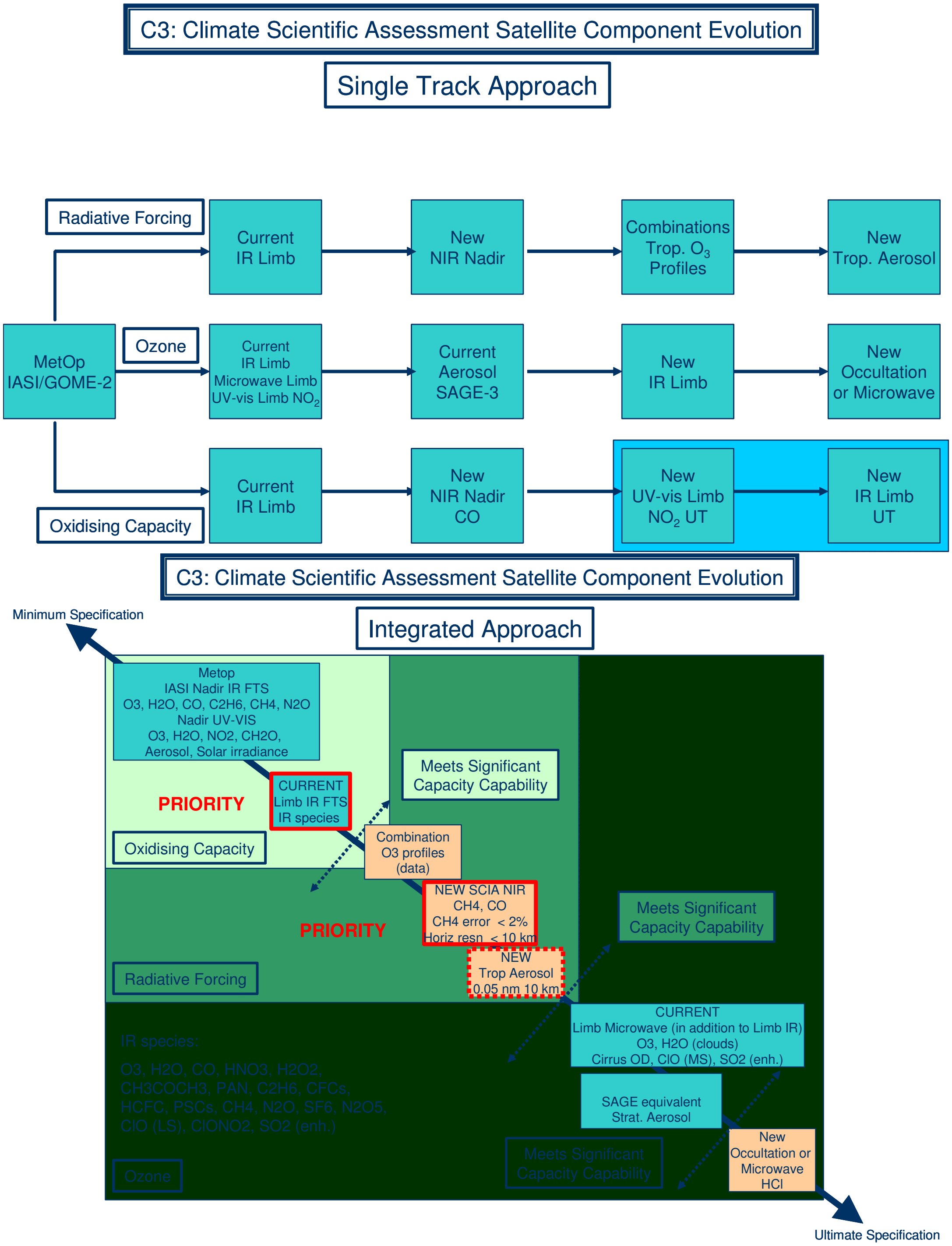

Figure 4.2.3.4 - C3 specification diagram. Two approaches to achieving the objectives are illustrated, one taking a single-track approach for each driver simultaneously, the other an integrated approach, achieving the oxidising capacity requirements first, then radiative forcing, and finally ozone.

Future Requirements

C1 and C2

Looking towards the future, there is a requirement to asses the potential of GEO measurements of GHGs from space. Fast time resolution measurements may provide a way to increase precision.

Table 4.2.3.1 – Consolidated requirements for climate mission focussed on emission of GHG monitoring (data merge of all satellite requirements from Chapter 2) for C1S and C2S.

Requirement / Data Product	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
CO_2 (PBL sensitive)	Trop. column	10 / 50	--	6 / 12	0.5%
	Total column	10 (1) / 50 (20)	--	6 (1) / 12	0.5 (2) %
	PBL	5 / 50	--	6 / 12	10%
	MS	50 / 200	1 / 3	12 / 24*7	10%
	US	50 / 200	1 / 3	12 / 24*7	10%
CH_4 (PBL sensitive)	Trop. column	10 / 50	--	24 / 24*3	2%
	Total column	10 / 50	--	24 (12) / 24*3	2%
	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 200	1 / 3	12 / 24*3	20%
O_3	Troposphere	10 / 50	2 / 5	12 / 24*3	20%
	Tropospheric column	10 / 50	--	12 (6) / 24*3	25%
	Total column	50 / 100	--	24 (6) / 24*3	3 (5) %
	PBL	5 / 50	--	6 / 24	30%
	LS	50 / 100	0.5 / 2	6 / 24*3	10%
	MS	50 / 200	1 / 3	6 / 24*7	20%
	US+M	50 / 100	3 / 5	6 / 24*7	20%
NO_2 (PBL sensitive)	Troposphere	10 / 50	2 / 5	12 / 24*3	50%
	Tropospheric column	10 / 50	--	12 / 24*3	$1.3 \cdot (10)15$ cm^{-2}
	Total column	10 / 50	--	12 / 24*3	$1.3 \cdot (10)15$ cm^{-2}
CO (PBL sensitive)	Troposphere	10 / 50	2 / 5	12 / 24*3	20%
	Tropospheric column	10 / 50	--	12 / 24*3	25%
	Total column	10 / 50	--	12 / 24*3	25%
Aerosol OD	PBL	5 / 10	--	1 / 6	0.05
	Troposphere	10 (5) / 50	--	6 (3) / 24*3 (24)	0.05
	LS	50 / 100	1 / part. column	12 / 24*3	0.05
	MS	50 / 200	2 (1) / part. column	12 / 24*3	0.05
	Total column	10 / 50	--	12 / 24*3	0.05
Aerosol absorption OD	PBL	5 / 10	--	1 / 6	0.01
	Troposphere	10 (5) / 50	--	6 (3) / 24*3 (24)	0.01
	Total column	10 / 50	--	6 / 24*3	0.01
H_2O	PBL	5 / 50	--	1 / 6	50%
	FT	10 / 50	0.5 / 2	1 / 6	30%
	UT	10 / 100	0.5 / 2	1 / 6	30%
	LS	50 / 100	0.5 / 2	3 / 24	20%
	MS	50 / 200	1 / 3	6 / 24*7	20%
	US	50 / 200	3 / 5	6 / 24*7	20%
	Total column	10 / 50	--	6 / 24*3	5%
N_2O	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 200	1 / 3	12 / 24*3	20%
	US	50 / 200	3 / 5	12 / 24*3	20%
	Total column	10 / 50	--	12 / 24*3	2%
Cirrus OD	UT	50 / 100	--	6 / 24	100%
SF_6	LS	50 / 100	1 / 3	12 / 24*7	10%
	MS	50 / 200	1 / 3	12 / 24*7	10%
	US	50 / 200	3 / 5	12 / 24*7	10%
HDO	LS	50 / 100	1 / 3	12 / 24*7	10%
	MS	50 / 200	1 / 3	12 / 24*7	10%
	US	50 / 200	3 / 5	12 / 24*7	10%
HF	LS	50 / 100	1 / 3	12 / 24*7	10%
	MS	50 / 200	1 / 3	12 / 24*7	10%
	US	50 / 200	3 / 5	12 / 24*7	10%
Aerosol phase function	PBL	5 / 10	--	1 / 6	0.1 on asymmetry factor
	Troposphere	5 / 50	--	3 / 24	
Cirrus phase function	UT	10 / 100	--	6 / 24	0.1 on asymmetry factor

(C2S- requirement)

Requirements can be met by current instruments

Some requirements met

No requirements met

C3S

The requirements for C3 are extensive but can broadly be divided into three areas: 1) radiative forcing and emissions; 2) oxidising capacity and 3) recovery of the stratospheric ozone layer. This is an essential step in order to match requirements and potential system elements directly.

Table 4.2.3.2 – Consolidated requirements for climate mission focussed on emission of GHG monitoring (data merge of all satellite requirements from Chapter 2) for C3S separated into main driver

Radiative forcing

Requirement / Data Product	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Troposphere UT	10 / 50 20 / 100	1 / 3 0.5 / 2	6 / 24*3 6 / 24*3	30% 20%
H_2O	PBL Troposphere UT	1 / 20 10 / 50 20 / 100	-- 1 / 3 0.5 / 2	6 / 24 6 / 24*3 6 / 24*3	30% 30% 20%
CO_2	MS Total column	50 / 100 10 / 50	2 / 3 --	12 / 24*3 1 / 12	10% 0.5%
CH_4	Total column	10 / 50	--	12 / 24*3	2%
N_2O	Total column	10 / 50	--	12 / 24*3	2%
Cirrus OD	UT	10 / 100	--	6 / 24	100%
PSC occurrence	LS	50 / 100	0.5 / 2	6 / 24*3	< 10% mis-assignments
AOD	PBL Troposphere Total column	5 / 20 10 / 50 10 / 50	-- -- --	6 / 24 6 / 24 12 / 24*3	0.05 0.05 0.05
Aerosol absorption OD	Troposphere Total column	5 / 50 5 / 50	-- --	6 / 24 6 / 24	0.01 0.01
Spectral solar irradiance	TOA	--	--	24 / 24*7	2%
CFC-11	LS MS Stratosphere	50 / 100 50 / 200 50 / 100	1 / 3 2 / 3 --	12 / 24*7 12 / 24*7 12 / 24*7	20% 20% 20%
CFC-12	LS MS Stratosphere	50 / 100 50 / 200 50 / 100	1 / 3 2 / 3 --	12 / 24*7 12 / 24*7 12 / 24*7	20% 20% 20%
HCFC-22	UT LS MS Stratosphere	20 / 100 50 / 100 50 / 200 50 / 100	1 / 3 1 / 3 2 / 3 --	12 / 24*3 12 / 24*3 12 / 24*3 12 / 24*3	20% 20% 20% 20%
SO_2 (enhanced)	Troposphere LS MS Total column	10 / 50 50 / 100 50 / 200 10 / 50	1 / 3 1 / 3 2 / 3 --	6 / 24*3 12 / 24*3 12 / 24*3 6 / 24*3	50% 50% 50% 50%
Aerosol phase function	Troposphere LS MS Total column	10 / 50 50 / 100 50 / 200 10 / 50	-- 1 / part. column 2 / part. column --	6 / 24 12 / 24*3 12 / 24*3 6 / 24	0.1 on asymmetry factor
Cirrus phase function	UT	10 / 100	--	6 / 24	0.1 on asymmetry factor

Oxidising capacity

Requirement / Data Product	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Tropospheric column	10 / 50	--	6 / 24*3	25%
H_2O	Trop. column	10 / 50	--	6 / 24*3	10%
CO	Troposphere Trop. column UT LS	10 / 50 10 / 50 20 / 100 50 / 100	1 / 3 -- 1 / 3 1 / 3	12 / 24*3 12 / 24*3 12 / 24*3 12 / 24*3	30% 25% 20% 20%
NO_2	Troposphere Trop. column UT	10 / 50 10 / 50 20 / 100	1 / 3 -- 1 / 3	6 / 24*3 12 / 24*3 6 / 24*3	30% $1.3 \cdot (10)15\ cm^{-2}$ 50%
CH_2O	Troposphere	10 / 50	1 / 3	6 / 24*3	30%

	Trop. column	10 / 50	--	12 / 24*3	1.3·(10)15 cm^{-2}
	UT	20 / 100	1 / 3	6 / 24*3	30%
	Total column	10 / 50	--	12 / 24*3	1.3·(10)15 cm^{-2}
HNO_3	Troposphere	10 / 50	1 / 3	6 / 24*3	30%
	UT	20 / 100	1 / 3	6 / 24*3	20%
	Total column	10 / 50	--	12 / 24*3	20%
H_2O_2	Troposphere	10 / 50	1 / 3	6 / 24*3	30%
	UT	20 / 100	1 / 3	6 / 24*3	30%
CH_3COCH_3	Troposphere	10 / 50	--	6 / 24*3	30%
	UT	20 / 100	1 / 3	6 / 24*3	30%
	Total column	10 / 50	--	6 / 24*3	30%
C_2H_6	Troposphere	10 / 50	--	6 / 24*3	50%
	UT	20 / 100	1 / 3	6 / 24*3	50%
	Total column	10 / 50	--	6 / 24*3	50%

Ozone

Requirement / Data Product	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	LS	50 / 100	0.5 / 2	6 / 24*3	20%
	MS	50 / 100	2 / 3	6 / 24*3	20%
	US+M	100 / 200	3 / 5	6 / 24*7	20%
	Total column	50 / 100	--	6 / 24*3	3%
H_2O	LS	50 / 100	0.5 / 2	6 / 24*3	20%
	MS	50 / 100	2 / 3	6 / 24*7	20%
	US+M	100 / 200	3 / 5	6 / 24*7	20%
	Total column?	50 / 100	--	6 / 24*3	10%
CH_4	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 100	2 / 3	12 / 24*3	20%
N_2O	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 100	2 / 3	12 / 24*3	20%
	US	50 / 100	3 / 5	12 / 24*7	20%
NO_2	LS	50 / 100	1 / 3	12 / 24*3	50%
	MS	50 / 200	2 / 3	12 / 24*3	30%
	Total column	50 / 100	--	12 / 24*3	10%
HNO_3	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 200	2 / 3	12 / 24*3	20%
AOD	LS	50 / 100	1 / part. column	12 / 24*3	0.05
	MS	50 / 200	2 / part. column	12 / 24*3	0.05
HCl	LS	50 / 100	1 / 3	12 / 24*3	20%
CH_3Cl	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 200	2 / 3	12 / 24*3	20%
	Stratosphere	50 / 100	--	12 / 24*3	20%
CH_3Br	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 200	2 / 3	12 / 24*3	20%
	Stratosphere	50 / 100	--	12 / 24*3	20%
SF_6	LS	50 / 100	1 / 3	12 / 24*7	10%
	MS	50 / 200	2 / 3	12 / 24*7	10%
	US	50 / 200	3 / 5	12 / 24*7	10%
HDO	LS	50 / 100	1 / 3	12 / 24*7	10%
	MS	50 / 200	2 / 3	12 / 24*7	10%
	US	50 / 200	3 / 5	12 / 24*7	10%
	Stratosphere	50 / 100	--	12 / 24*7	10%
HF	LS	50 / 100	1 / 3	12 / 24*7	10%
	MS	50 / 200	2 / 3	12 / 24*7	10%
	US	50 / 200	3 / 5	12 / 24*7	10%
N_2O_5	Troposphere	10 / 50	--	6 / 24*3	30%
	UT	20 / 100	1 / 3	6 / 24*3	30%
	LS	50 / 100	1 / 3	12 / 24*3	50%
	MS	50 / 200	1 / 3	12 / 24*3	50%
	Stratosphere	50 / 100	--	12 / 24*3	50%
PAN	Troposphere	10 / 50	--	6 / 24*3	30%
	UT	20 / 100	1 / 3	6 / 24*3	30%
	Total column	10 / 50	--	6 / 24*3	30%
ClO	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 200	2 / 3	12 / 24*3	20%
	Stratosphere	50 / 100	--	12 / 24*3	20%
$ClONO_2$	LS	50 / 100	1 / 3	12 / 24*3	20%
	MS	50 / 200	2 / 3	12 / 24*3	20%
	Stratosphere	50 / 100	--	12 / 24*3	20%

Requirements can be met by current instruments
Some requirements met
No requirements met

As only CO_2 and CH_4 are not in Table 4.2.2.1 recommend that some assessment of GEO to deliver these measurements is made.

Future Requirements

In summary, for GHG emissions (protocol monitoring)

- There are not enough data from current missions to assess the impact of space borne measurements for climate monitoring.
- With respect to routine monitoring, ground-based sites fulfil many of the requirements
- Clearly not a candidate for operational monitoring but there is an urgent requirement for the development of precursor missions

For assessment, there is a complex web of requirements, probably best served by a LEO limb-sounding mission that measures lots of things. There is some overlap with the requirements of ozone and UV.

4.3 Conclusion

There are three different areas at different levels of maturity

Ozone and UV - Many of the requirements for stratospheric O_3 and UV can be met by current/planned systems with respect to nadir measurements, there seems to be a hole with respect to operational limb monitoring of key trace species.

It is concluded that only the A1 theme requirements can be met by the planned Metop and ground-based systems. The other stratospheric A2 and A3 themes require limb sounding capabilities. For A2, only ozone profiles are mandatory but measurements of other species are highly desirable: ClO, polar stratospheric clouds, stratospheric aerosol, HNO_3, H_2O, tracers, and HCl. For A3, all the A2 measurements are required with, in addition, HCFCs, $ClONO_2$, and SO_2 (enhanced). A limb mid-infrared system is therefore suggested although a microwave system also has significant capabilities, particularly in cloudy regions of the atmosphere. An ultra-violet visible limb instrument (building on SCIAMACHY and GOMOS) can also monitor the important compounds of NO_2 and BrO.

For *Air Quality*, there is a need and requirement for a space-based system but the requirements/performance require a better quantitative basis. The implementation of a high time resolution, horizontal spatial resolution with optimal PBL information is required.

For air quality, it was shown that all systems (B1 to B3) were essentially similar with a prime requirement for high spatial (<20 km) and temporal (<2 hours) resolution measurements of O_3, CO, NO_2, SO_2, HCHO, and H_2O (B2/B3), with sensitivity to the PBL. Instruments are likely to be nadir ultra-violet/visible with shortwave infra-red or mid infra-red capability for CO. For B3 particularly, aerosol measurements at multiple wavelengths would enhance the system ideally in conjunction with nighttime measurements

Climate - For treaty monitoring and verification in respect of GHG, a better assessment of current and planned systems is required. There would be some benefit to looking at high time resolution measurements of GHG. Future monitoring of GHG from space is important.

Climate - For assessment and NRT climate, the overall requirements suggest a need for an operational limb monitoring mission. There is some need to prioritise the trace species requirements.

For operational use, there is requirement to analyse the clear sky bias of the measurement systems.

For climate, the C1 (protocol-monitoring) system was notably different to those for C2 and C3. Kyoto protocol-monitoring in C1 demands high precision measurements of CH_4 and CO (and CO_2) building on the shortwave infra-red measurements demonstrated by SCIAMACHY. Improved NO_2 measurements (spatial resolution of 10 km) would also be ideal. It is suggested that C1 systems could be combined with B1 to B3 systems at some point in the evolution of the GMES system. For C2 and C3, the priorities are limb sounder measurements for high vertical resolution (<2 km). For C2, measurements of H_2O, O_3, CH_4, and N_2O suggest either microwave or mid infra-red (building on MIPAS capabilities) limb whereas for C3, limb mid-infrared is more likely to be a priority to measure the large range of necessary species to monitor changes in radiative forcing, oxidising capacity and stratospheric ozone wth sensitivity also to the upper troposphere.

4.3.1 Overall Recommendations

With respect to a space segment of a measuring system for operational monitoring, it is clear there are three overall requirements that cannot be met by current or planned systems

- High temporal/spatial resolution space-based measurements of tropospheric (PBL) composition for application to AQ

- High vertical resolution measurements in the UT/LS region for application in ozone and climate applications
- High spatial resolution and high precision monitoring of climate gases (CH_4, CO and CO_2) and aerosol monitoring with sensitivity to the PBL

Implementation options should be investigated as part of this study.

With respect to the issue of greenhouse gas monitoring from space, there is a strategy and user requirement for this be further investigated. Given the time-lag with respect to the development of missions it would be dangerous to wait until OCO is proven.

Looking further into the future beyond operational monitoring, it is clear that the ideal space borne system would be able to provide vertical information throughout the depth of the atmosphere. Active systems have the potential in the longer term to provide this for a number of chemical species and aerosol.

5 The geostationary component of an operational atmospheric chemistry monitoring system: Specification and expected Performance

5.1 Introduction

5.1.1 Analysis of relevant user requirements from WP2300

User requirements driving the specification of a geostationary component of an operational atmospheric chemistry mission are mainly coming from the area of Air Quality applications (B1S - B3S), because of the demanding requirement on the revisit time (see Chapter 4 (WP 2300) recommendation (a)).

Parameter	Application Area				Uncertainty	Horizontal Resolution	Vertical Resolution Troposphere	Revisit Time
	AQ	C	UV-VIS-NIR	TIR		[km]	[km]	[hours]
O_3	X		X	X	10 – 25 %	5 – 20	1-3 - TrC	0.5 - 2
NO_2	X		X		10 – 30 % (1.3e15mol/cm^2)	5 – 20	1-3 - TrC	0.5 – 2
CO	X		X	X	20 – 25 %	5 – 20	1-3 - TrC	0.5 – 2
SO_2	X		X		20 – 50% (1.3e15mol/cm^2)	5 – 20	1-3 - TrC	0.5 – 2
HCHO	X		X		20 – 50% (1.3e15mol/cm^2)	5 – 20	1-3 - TrC	0.5 – 2
Aerosol Optical Depth	X	X	X		0.05	5 – 20	-	0.5 – 2
Aerosol Type	X		X	X	< 10% mis-assignments	5 – 20	-	0.5 – 2
H_2O	X	X	X	X	10 – 20 %	5 – 20	1-3- TrC	0.5 – 2
HNO_3	X			X	20 % (1.3e15mol/cm^2)	5 – 20	1-3 – TrC	0.5 – 2
N_2O_5 (night)	X			X	20 – 50% (1.3e15mol/cm^2)	5 – 20	1-3 - TrC	0.5 – 2
PAN	X			X	20 % (1.3e15mol/cm^2)	5 – 20	1-3 - TrC	0.5 - 2
Organic Nitrates (B3-S only)	X			X	30 %	5 – 20	PBL only	0.5 - 2

Table 5.1: *Summary of Level 2 requirements on tropospheric measurements (TrC: Tropospheric Column) derived from Chapter 4 (WP 2300) with revisit time requirement of < 2 hrs.*

Common to all requirements in the areas B1-S and B2-S is the requirement to determine tropospheric concentrations in combination with a revisit time of 0.5 – 2 hrs. The main requirement not addressed with existing and planned missions is the revisit time requirement of 0.5 – 2 hours (see Chapter 4).
As detailed in Chapter 3, the coverage requirement for the air quality theme is driven by its focus on local, regional and continental scale environmental air quality issues. The threshold coverage requirements for operational applications directed to EU policy, is therefore the European continent, including Turkey, and Europe’s surrounding coastal waters as well as the closest parts of the North-Atlantic, which typically impact on the boundary layer in Europe by long-range transport (see Chapter 3).
For the regional coverage requirement (threshold) already one GEO system is able to cover the European continent and surrounding areas and in Chapter 7 (WP3300) it was concluded that the geostationary orbit is the optimum with respect to the applications requiring short revisit times and coverage of Europe.

This report will therefore focus on the derivation of mission and instrument requirements for the GEO component of an operational atmospheric chemistry mission to address user requirements as given above.

5.1.2 Complementarity and Synergism of Atmospheric Chemistry Measurements from GEO and LEO

Satellite sounding instruments generally employ one of two types of viewing geometry, i.e. *nadir* viewing or *limb* viewing. Nadir viewing instruments observe a selected solid angle centred about a given spot on the Earth. Spatial coverage is maintained by a scanning and/or imaging systems.
Limb viewing instruments scan vertically the earth's atmosphere, observing large horizontal paths at different altitudes. Limb viewing generally yields high vertical resolution and ability to observe higher in the atmosphere than nadir sounding instruments. At low altitudes, the horizontal resolution of the limb observation is often limited. Therefore, limb observations have been primarily used for sounding the mesosphere and stratosphere down to the tropopause region. For a geostationary orbit the use of a limb sounding instrument is of no significant use because of the extremely limited coverage. For geostationary applications therefore only nadir sounding instruments are further investigated. Nevertheless, for a global atmospheric observing system a combination of atmospheric limb sounding measurements from LEO and nadir sounding measurements from geostationary orbit is required.

Low earth orbit and geostationary platforms have distinct advantages and disadvantages with respect to sampling: geostationary orbiting instrumentation providing high spatial and temporal resolution with up to hemispheric coverage. Near global coverage necessitates 3-4 geostationary platforms. LEO platforms have clear advantages with respect to vertical resolution, polar and global coverage, especially for limb sounding applications sensing the upper troposphere, stratosphere and mesosphere.

In contrast to that, a geostationary orbit offers the following general advantages:

- Up to an order of magnitude more cloud free observations/day/location due to a factor of 10-20 more frequent observation (compared to sun-sync. LEO)
- Synoptic picture of a large area (up to 1/4 of the Earth) every 30 - 60 min.
- Regional Coverage with high spatial resolution (5 km x 5 km)
- Observation of spatial-temporal variability and diurnal variation of parameters
- Observation as function of solar illumination/scattering angle
- Observation of short-lived and unpredictable events like accidental releases of pollutants, lightning, volcanic eruptions, and fires
- Accurate and complete statistics of events in one hemisphere.

Sensors in a geostationary orbit are optimal for closing the gap between the different spatial (regional to continental) and temporal scales (short term to long term). A very important advantage in the context of tropospheric measurements is the roughly order of magnitude higher number of cloud free observations per day and geo-location due to a factor of 10-20 more frequent observations per day in comparison to a measurements from LEO.
It was quantified within this study how many cloud free observations per day per geolocation are typically available from geostationary orbit, depending on the IFOV. The analysis is based on MVIRI/METEOSAT imager data. An instrument with 5 x 5 km^2 (SSP) in GEO will deliver over Europe on average approx. 2 (winter) to 8 (summer), (seasonal average: 5) cloud free observations per day per geo-location, based on MVIRI cloud statistics. An instrument with 15 x 15 km^2 (SSP) in GEO will deliver over Europe on average approx. 1.5 (winter) to 6.5 (summer), (seasonal average: 3.5) cloud free observations per day per geo-location, based on MVIRI cloud statistics. In comparison, a METOP and NPOESS instruments in LEO allow for 0.2-0.3 cloud free observation, which can nearly doubled by adding a 10 km x 10 km instrument in LEO.

A geostationary orbit is therefore optimal for monitoring and forecasts of short-term temporal and spatial variability of tropospheric processes and events, as required for example for the regional Air Quality applications.

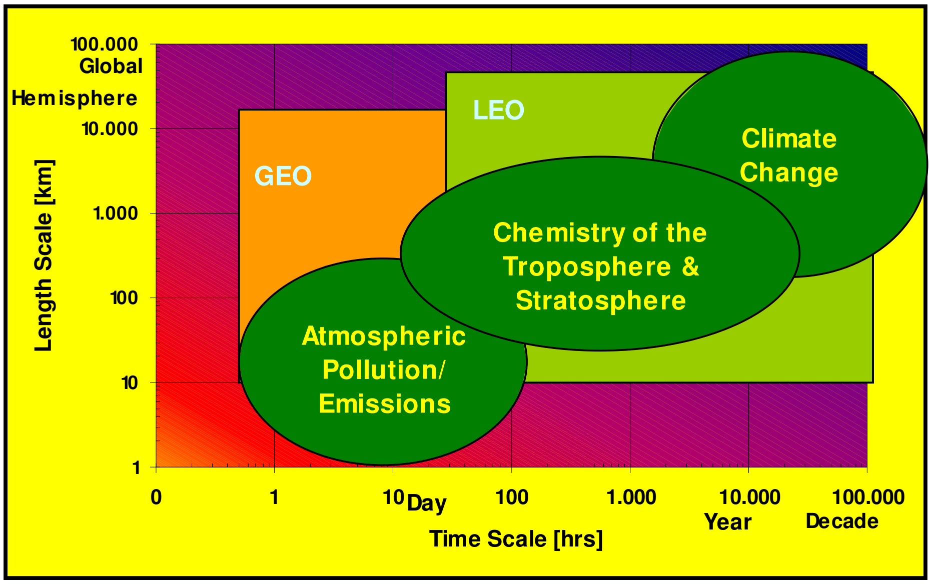

Figure 5.1 *Scales of atmospheric processes in comparison to the scales covered by LEO and GEO systems. Omitted is the vertical scale.*

In addition to the advantages of a geostationary with respect to certain applications, there exists also important synergies between GEO and LEO. For example the global characterisation of the composition of the stratosphere by limb sounders in LEO can be used, in combination with data assimilation techniques, to constrain the determination of tropospheric trace gas measurements from GEO for those gases with significant concentrations above the tropopause, for example O_3 and NO_2.

5.1.3 Scope

Within this report the Level-2 requirements given above will be translated to mission and instrument specifications as input for an assessment of the instrument concepts (Chapter 7, WP 3300). The requirements on horizontal resolution, revisit time and coverage can directly translated to specifications with respect to the Field-of-View, the horizontal resolution and the revisit time of the measurements. The overall approach is summarised in Section 5.2.

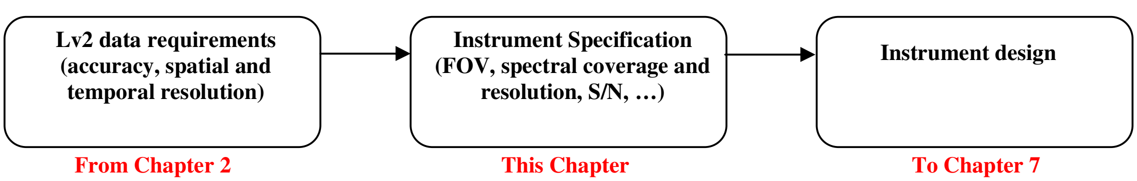

Figure 5.2: *Study logic.*

Beside the requirements on horizontal resolution, revisit time and coverage, the specification is driven by the measurement technique used to derive the relevant parameter taken into account. Within this Chapter (WP3100) two measurement techniques to derive the geophysical parameters are investigated: the absorption spectroscopy of solar back scattered radiation and the thermal infrared emission spectroscopy.

Backscattered Solar (UV, VIS, NIR, SWIR) radiation penetrates deep into the troposphere and will reach the Earth surface if not interfered with by clouds. GOME and SCIAMACHY measurements have demonstrated that total columns (including the PBL) of O_3, NO_2, SO_2, BrO, OClO, HCHO, H_2O, CO, CH_4, CO_2, UV-A, UV-B, cloud and aerosol parameters can be successfully retrieved from the nadir UV-VIS-NIR-SWIR spectra. Solar backscatter measurements are sensitive to the tropospheric column including the PBL, but height resolved information in the troposphere is typically not directly derived, but can be indirectly derived by cloud slicing and assimilation techniques. Tropospheric column amounts (including the PBL) have been shown to be retrievable from GOME and SCIAMACHY nadir spectra for the species O_3, NO_2, BrO, and HCHO. UV-SWIR observations yield total and tropospheric column amounts and/or vertical information on O_3, CO, CH_4, H_2O, CO_2, NO_2, SO_2, HCHO, BrO, UV-A and UV-B, cloud and aerosol parameters. Section 5.3 therefore focuses on instrument specification to derive tropospheric columns of O_3, NO_2, CO, H_2O, SO_2, and HCHO from solar backscatter measurements.

The emission of thermal infrared (TIR) radiation contains information on trace constituents in the troposphere and the stratosphere. TIR radiation is sensitive to tropospheric trace gas concentrations with a weighting towards the free troposphere and rapidly decreasing sensitivity in the lowest troposphere and PBL. Retrieval of tropospheric column data down to the surface from mid-IR measurements is often not possible due to the lack of sensitivity of the IR measurements below the free troposphere [Clerbaux et al., 2003b]. Nevertheless mid-IR measurements yield important information in the mid and upper troposphere [Clerbaux et al., 2003a]. TIR measurements can be observed both during day and night. This was successfully demonstrated by the nadir viewing ADEOS IMG instrument, and similar data retrieval schemes are used for the NASA EOS-Aura instrument TES and will be used for the EUMETSAT MetOp instrument IASI. TIR observations yields vertical profile information on O_3, CO, CH_4, H_2O, N_2O and tropospheric column amounts on PAN, C_2H_6, SO_2 (enhanced conditions), HCHO (enhanced conditions) and CFCs. Section 5.4 focuses on instrument specifications to derive tropospheric profile data for O_3, H_2O and CO and tropospheric column data for SO_2, CH_2O, HNO_3, N_2O_5 (night) and PAN from TIR measurements.

5.2 Measurement Technique Independent Specifications

5.2.1 Field of View, Instantaneous Field of View and Temporal Coverage

For the geometrical specifications, we have assumed a geostationary instrument pointing off-Nadir to the North-East towards Europe and we have used the CHIMERE chemical model to assess the impact of pointing accuracy, stability and knowledge. This is considered to be representative for the threshold requirements for Air Quality.

The **field of view (FOV)** is defined by the coverage. As detailed in Chapter 2 (WP2100), the threshold coverage requirement for the air quality theme is driven by its focus on local, regional and continental scale environmental air quality issues. The threshold coverage requirements for operational applications directed to EU policy, is therefore the European continent, including Turkey, and Europe's surrounding coastal waters as well as the closest parts of the North-Atlantic, which typically impact on the boundary layer in Europe by long-range transport. This translates into the following approximate latitude-longitude boundaries of the FOV: N-S: 30°N – 65°N; E-W: 30°W – 45°E (@40°N). A satellite position centred in E-W direction over the target area is preferred.
In addition to the area which needs to be covered by the data products, coverage of the Sahara is required as a reflectance calibration target (GOME, MERIS, SCIAMACHY, SEVIRI experience). The expected frequency of this vicarious calibration is weekly to monthly.

The **instantaneous field of view (IFOV)** is primarily defined by the horizontal resolution requirement (5 – 20 km). In addition, as the focus of the required observations is the troposphere including the PBL, another aspect for IFOV specification is the optimisation of the IFOV w.r.t. minimisation of cloud contamination. For a 20 km x 20 km the percentage of cloud free scenes is around 10 % and increases to over 30 % for a 5 km x 5 km ground pixel. In addition, it was assessed within this study how many cloud free observations per day per geo-location are typically available from geostationary orbit, depending on the IFOV. The analysis is based on MVIRI imager data (see Annex A). An instrument with 5 x 5 km^2 (SSP) in GEO will deliver over Europe on average approx. 2 (winter) to 8 (summer), (seasonal average: 5) cloud free observations per day per geo-location, based on MVIRI cloud statistics. An instrument with 15 x 15 km^2 (SSP) in GEO will deliver over Europe on average approx. 1.5 (winter) to 6.5 (summer), (seasonal average: 3.5) cloud free observations per day per geo-location, based on MVIRI cloud statistics.

As the solar backscatter instrument has a higher sensitivity down to the lowest troposphere, it is for the solar backscatter instrument more important to reach the 5 km x 5 km IFOV than for the IR instrument.

The temporal coverage is defined by the revisit time requirement. The requirement was to have hourly data.

5.2.2 Pointing Stability and Knowledge

In order to evaluate the requirements on pointing stability and spatial knowledge, simulations with the CHIMERE [Menut 2003] chemical model (covering Europe) were carried out. Note that this approach is entirely independent of the measurement technique. The results are:

- The geo-location of the individual pixels must be known with a precision of better than 2 km (2σ) for a pixel size of 15-20 km, i.e. to about 10-20% of pixel over Europe, in order to limit the errors for the chemical assimilation of species with strong concentration gradients due to re-sampling of the data.
- The relative error is more important in regions where the concentrations are smaller (less polluted regions).

It was explicitly checked that the differences between the true tropospheric columns and those obtained after applying the shift are not affected by the limited resolution of the model.
One can conclude that for all these species, a shift of 1 km induces relative errors in the range between -20% et and +20 %. To illustrate the effect of larger shifts (2.5 km and 5 km) the results for O_3 and NO_2 are shown in ***Figure 5.1*** (CHIMERE run at regional scale; pixel size 0.25° (shifts are indicated). Shifts of 2.5 km and more lead to higher errors (especially for NO_2). It has to be noted that this requirement is depending on the characteristics of the geophysical parameter of interest. As given above, NO_2 for example is much more sensitive to the geo-location knowledge than O_3.

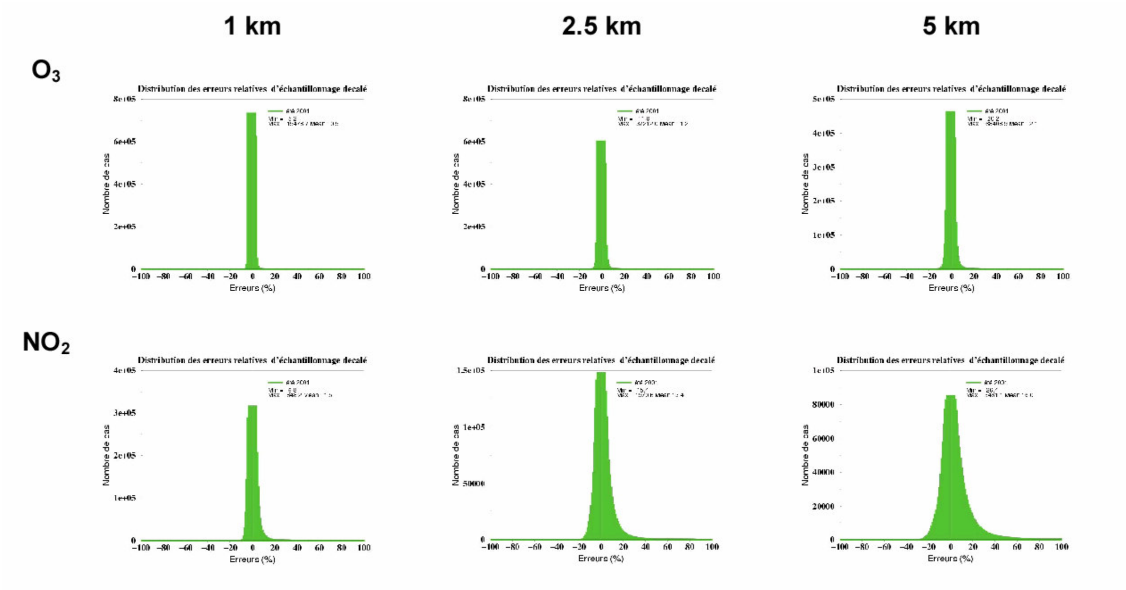

Figure 5.1: *Impact of 1, 2.5 and 5 km shift due to pointing accuracy for O_3 and NO_2.*

5.3 UV-VIS-NIR Instrument Specification

5.3.1 Measurement Techniques and Assessment of Relevant Error Sources

5.3.1.1 Aerosol Retrieval

User requirements on Aerosol (AOT and aerosol type) over land needs moderately to low spectrally resolved data on the TOA spectral reflectance of the Earth combined with surface spectral reflectance, polarimetric and/or multi-angular data. Various algorithms have been and are being developed for the retrieval of aerosol information from radiance measurements. The main difficulty in space-borne aerosol retrieval consists in the separation of land or sea surface effects from atmospheric aerosol effects. Currently the following methods are in use: (1) Veefkind et al.1998, 1999 developed algorithms for multi-angle viewing techniques as it is possible for ATSR-2, AATSR and MISR. (2) Torres et al. 1998, 2001 used the UV absorption and adequate aerosol models for the determination of the absorbing aerosol index (AAI) and the UV aerosol optical thickness with TOMS, based on a long-term climatology of the spectral surface reflectance. (3) Guzzi et al. 1997 tries a model based estimation for GOME, which also require a climatology. In all climatology based retrievals the quality of the aerosol retrieval depends on the quality of the climatological data data. (4) Kaufman et al. 1997 applies the dark-target method, based on cross-correlations of IR channels (2.2 µm) and short-wave channels to separate the aerosol properties. (5) Von Hoyningen-Huene et al. 2002 developed a method, estimating the required ground properties by a linear mixing of different surface spectra from the NDVI. (6) Deuze et al. 2000 applies on POLDER data for the separation the different polarization properties between atmospheric aerosol and ground. (7) Stam 2000 use polarisation measurements of GOME to establish aerosol type and size distribution. (8) Aerosol layer height can be determined from high resolution O_2-A band absorption spectra [Stephens and Heidinger 2000].
For remote sensing of aerosol from geostationary orbit it is proposed to combine polarimetric with spectral TOA albedo measurements from 350 nm to 1000 nm and also include limited multi-angular view (limited by temporal resolution from GEO). Simulations by O. Hasekamp indicate that with this type of measurements the AOT for fine and coarse mode aerosol can be determined.

5.3.1.2 Tropospheric Trace Gas Measurements

As the primary focus of the user requirements on a geostationary atmospheric chemistry mission is the determination of tropospheric distributions of trace gases, a brief overview is given about the techniques to derive tropospheric information from nadir UV-VIS-NIRSWIR solar backscatter measurements. Three different categories of trace gases have to be discussed, namely those (1) where the majority of the total atmospheric amount resides in the troposphere with a concentration peak towards the boundary layer (e.g. CO, HCHO, SO_2, H_2O), those (2) where the column amount in the troposphere and stratosphere is typically comparable (e.g. NO_2 under moderate to high polluted conditions), and those (3) where the stratospheric amount is dominating the total column concentration (e.g. O_3).
For constituents, where the majority of the atmospheric amount resides in the lower troposphere (e.g. CO, HCHO, SO_2, H_2O), the total column derived from UV, visible, NIR or SWIR solar backscatter measurements directly represents the tropospheric column amount including the boundary layer (under cloud free conditions).
Where column amounts in the troposphere and stratosphere are comparable (e.g. NO_2) or, the stratospheric amount is dominating the total column (e.g. O_3), techniques needs to be applied to separate tropospheric and stratospheric concentrations. This can be done in case of nadir sounding measurements by estimating the stratospheric column concentration and remove the stratospheric column from the total column measurements yielding the tropospheric column. A variety of techniques have been developed to achieve this objective.
The measurement principle has been demonstrated successfully for several instruments on platforms in sun-synchronous LEO (e.g. TOMS, GOME, SCIAMACHY, references see table below). ***Table 5.2*** is

summarising the reported error estimates for tropospheric trace gas retrievals This table gives an overview of relevant and dominating error sources and gives also some guidance where it is worthwhile to improve instrument specification or the retrieval methodology to meet usser requirements.

Tracegas Tropospheric Column Errors			total error	total error	SNR & Rad.	FWHM	AOT	Surface Albedo	Clouds
	Reference	Instrument	cloud free	incl. clouds	error	error	error	error	error
O3	Hudson et al.1998	TOMS TTO	10 -20						
	Ziemke et al. 1998	TOMS CCD	10 - 20						
	Valks et al. 2003	GOME CCD	10 - 20						
	Coldewey-Egbers et al. 2003	GOME WF-DOAS	12	19	3	2	5	10	15
	Liu et al. 2005	GOME OE, Validation		13 - 27					
NO2	Martin et al. 2001	GOME	36	41	3	2	20	30	20
	Richter et al. 2002	GOME	43	48	3	2	35	25	20
	Heland et al. 2002	GOME	26	28	3	2	18	18	10
	Boersma et al. 2004	GOME	23	34	3	1	20	10	25
	Heue et al. 2005	SCIAMACHY Validatio	20						
CO	Buchwitz et al. 2004	sensit./SCIAMACHY	21	24	15	15	2	2	10
	Buchwitz et al. 2005	SCIAMACHY Validatio	10 - 20						
HCHO	Wittrock et al 2000	GOME	30	30	5	2	0	30	0
	Palmer et al. 2002	GOME	41	42	30	20	20	0	10
	Ladstätter et al 2003	GOME	50	58	25	2	35	25	30
SO2	Eisinger et al 1998	GOME	36	36	30	0	20	0	0
H2O	Noel et al. 2004	SCIAMACHY	9	13	4	3	5	5	10
	Lang et al. 2003	GOME	18	21	10	5	10	10	10
	Noel et al. 2005	SCIAMACHY Validation		10 - 20					

Table 5.2: *Overview of tropospheric measurements in the solar backscatter and summary on error sources for tropospheric columns.*

From the table and the references given there the error on currently published tropospheric column measurements is dominated by three error sources: 1. errors of up to 20-30% due to unknown aerosol (AOT, height of aerosol layer), 2. errors of up 20-30% due to imperfect knowledge of the surface albedo, and 3. errors of up to 20-30% due to imperfect knowledge on clouds (fractional cloud cover, cloud top height, cloud optical thickness). Reported instrumental errors from instrument noise and non-optimum spectral resolution/sampling are ranging from well below 5% for O_3, NO_2 and H_2O up to 20%-30% for HCHO and SO_2. Other error sources to be taken into account are systematic biases due to absorption cross section errors and the uncertainty in the determination of the stratospheric column. Especially the latter is taken into account in this study by varying the error of the stratospheric column to estimate the impact on the retrieved tropospheric column explicitly. It has already been demonstrated by Boersma et al. [2004] (and references therein) in the case of tropospheric NO_2, by Noel et al. [2004] in the case of H_2O, and by [Coldewey-Egbers et al.] in case of O_3, that the impact of cloud and aerosol uncertainties can be minimised by the determination of the reflection and scattering characteristics of the observed ground scene by measuring the absorption of well mixed gase like O_2 or O_4 in parallel to the trace gas of interest. Efficient techniques to minimise errors due to clouds and aerosol are therefore already in place and tested.

W.r.t. the goal of the CAPACITY project it can be concluded based on the currently published error budgets, that beside the instrument related error sources, also the errors introduced by an imperfect knowledge of scene dependent parameters like surface albedo, aerosol and clouds needs to be controlled. Minimisation of these error sources needs therefore taken into account when specifying a mission. The instrumental error needs to be minimised by an appropriate instrument specification. The scene dependent errors needs to be minimised by adequate measurement strategy w.r.t. ground albedo, clouds, aerosol and stratospheric trace gas concentration amount. Especially w.r.t. ground albedo, clouds and aerosol information on the optical path length in the troposphere is required, which is estimated from absorption measurements of absorbers with well known height distribution (for example O_2, or the collision complex O_2-O_2). Relevant spectral windows needs to be included in the instrument specification.

5.3.2 Solar Backscatter Instrument Specifications

5.3.2.1 Spectral Coverage

The spectral areas in the UV-Vis-SWIR part of the backscattered solar spectrum should cover windows were the target parameters (O_3, NO_2, CO, H_2O, SO_2, CH_2O as well as AOT and relevant cloud and aerosol parameter) can be detected via their characteristic absorption or scattering characteristics. The number of spectral bands describes how many spectral regions are covered by the instrument.

Wavelength Range		Relevant Atmospheric Species	Products	Priority
Min [nm]	Max [nm]			
290	310	O_3	Stratospheric O_3 Column	A
310	400	O_3, SO_2, H_2CO, NO_2, BrO, Fraunhofer Lines, aerosol, surface	Total and trop. O_3, SO_2, HCHO, O_4, AAI, SSA, AOT(UV), surface albedo, CTH (Ring)	A
400	610	NO_2, O_3 (Chappuis), H_2O, O_4, aerosol, surface	NO_2, O_3, CTH, AOT(Vis) , surface albedo	A
755	780	O_2 A-band, surface	ALH, CTH, COT, AOT(NIR), surface albedo	B
2345	2375	CO, CH_4 surface	CO, AOT (SWIR), surface albedo	A/B

Table 5.3: *Summary of Spectral Coverage Requirements*

Main purpose of the O_2 A channel (755 – 780 nm) with its high spectral resolution is to estimate a mean aerosol layer height, as investigated by Rozanov and Timofeev 1994, Timofeev et al. 1995, Koopers et al. 1997, Heidinger 1998 etc.. The aerosol layer height (ALH) is important to quantitatively determine tropospheric trace gas concentrations under polluted conditions. As aerosol from pollution is mostly concentrated within the PBL [Ansmann et al. 2002, Wandlinger et al. 2002] the aerosol effect on nadir observations is from that height region. As an alternative to the estimate of the ALH from O_2 A-band absorption measurements, it might therefore be an option to use the boundary layer height from meteorological analysis as an aerosol layer estimate. Boundary layer height can be estimated for example from analysing meteorological fields w.r.t. a temperature inversion. The O2-A band channel with high spectral resolution is therefore priority B. Cloud top height and optical thickness can be determined alternatively from low spectral resolution (approx. 0.5 nm) O_2 A-band measurements. An O_2-A channel with spectral resolution of approx. 0.5 nm is therefore ranked as “A”.

CO can be detected in the thermal IR and the SWIR. The overall sensitivity to CO is higher in the IR than in the solar backscatter SWIR. Weighting functions in the SWIR show good sensitivity to boundary layer. Sensitivity to boundary layer CO in the IR depends mainly on the thermal contrast and the spectral resolution. For high spectral resolution nadir IR sounders like IMG or TES, the IR can also contribute to the lower tropospheric concentrations [Barret et al. 2005]. Nevertheless, SWIR will add to IR a factor of approximately two higher boundary layer sensitivity (Bovensmann et al. 2002, EUMETSAT MTG CO Study). The CO window proposed to be used in the SWIR here is driven by the fact that it contains 3 CO lines nearly free of other trace gas interference. To further minimise the

CH_4 and H_2O interference with CO, the window is somewhat enlarged. It will therefore also yield quantitative information on CH_4. For a combined solar backscatter TIR mission the CO channel has priority A/B depending on the spectral resolution of the IR instrument. In case the IR instrument reaches boundary layer sensitivity due to high spectral resolution, the SWIR channel might be ranked "B". For a UV-Vis-SWIR mission the CO channel is mandatory, as CO is requested by the user.

5.3.2.2 Spectral Resolution

The spectral resolution should be high enough to distinguish unambiguously all absorption, emission or scattering features of the species to be observed. Electronic transitions between rotational-vibrational levels of diatomic molecules often exhibit narrow absorption lines that require a moderate to high spectral resolution. High spectral resolution also allows for many spectral observations containing redundant information about surface and atmospheric conditions, which can be utilised together to reduce the effective noise of the set of observations and further improve the accuracy of the soundings in the boundary layer. This is especially important for the retrieval of scattering height and cloud information from O_2-A band absorption and the precise retrieval of H_2O and CO. To derive aerosol height resolved information in the troposphere (means scattering height), the spectral resolution in O_2 A-band should be improved in comparison to GOME and SCIAMACHY to better than 0.1 nm.
The table below summarises for the different spectral ranges and the requirements on spectral resolution.

Wavelength Range		Spectral Resolution (Resolving Power)
Min [nm]	Max [nm]	FWHM [nm]
290	310	< 1 (>400)
310	400	< 0.5 (>700)
400	610	< 0.7 (>700)
755	780	< 0.5 (>1500) A < 0.1 (>7800) B
2345	2375	< 0.1 (>23500)

Table 5.4: *Summary of Spectral Resolution Requirements*

5.3.2.3 Radiometric Resolution (SNR) for the radiance measurements

The radiometric resolution is specified in term of signal-to-noise (SNR) associated to a reference radiance (see table) at which the SNR is computed.
The reference radiance is calculated with MODTRAN (s/c at geostationary distance, observed region at 55°N, fall equinox, 12 LT, 1976 US standard atmosphere, UV-Vis: albedo 0.3, SWIR: albedo 0.1, tropospheric/background stratospheric aerosol, no cloud, no precipitation). The maximum and minimum radiance are also calculated with MODTRAN (same conditions but for maximum observed region at 0°N and albedo 1.0 and for minimum ground point at lat. 55°N, long 0° with ground albedo 0.01).

Wavelength [nm]	Minimum Radiance [photons/(cm^2 s sr nm]	Reference Radiance [photons/(cm^2 s sr nm]	Maximum Radiance [photons/(cm^2 s sr nm]	Signal-to-Noise
290	5 E+10	6 E+10	7 E+10	100
300	1 E+11	1.1 E+11	1.7 E+11	300
305	3.3 E+11	3.5 E+11	2.0 E+12	500
312	1.9 E+12	2.0 E+12	1.0 E+13	1000
320	6.8 E+12	7.3 E+12	2.3 E+13	1500
350	1.4 E+13	1.9 E+13	5 E+13	1800
450	1.8 E +13	3.8 E +13	1.5 E+14	2500
550	1 E+13	3.1 E+13	1.5 E+14	2500
700	5.5 E+12	2.8 E+13	1.5 E+14	2000
775	4.5 E +12	2.6 E +13	1.5 E+14	2000
2350	1 E+11	1 E+12	1 E+13	200

Table 5.5: *Summary of radiance SNR Requirements (per FWHM). Maximum radiance is specified to avoid saturation.*

Wavelength [nm]	Minimum Radiance [photons/(cm^2 s sr nm]	Reference Radiance [photons/(cm^2 s sr nm]	Maximum Radiance [photons/(cm^2 s sr nm]	Signal-to-Noise
290	5 E+10	6 E+10	7 E+10	100
300	1 E+11	1.1 E+11	1.7 E+11	300
305	3.3 E+11	3.5 E+11	2.0 E+12	500
312	1.9 E+12	2.0 E+12	1.0 E+13	1000
320	6.8 E+12	7.3 E+12	2.3 E+13	1500
350	1.4 E+13	1.9 E+13	5 E+13	1800
450	1.8 E +13	3.8 E +13	1.5 E+14	2500
550	1 E+13	3.1 E+13	1.5 E+14	2500
700	5.5 E+12	2.8 E+13	1.5 E+14	2000
775	4.5 E +12	2.6 E +13	1.5 E+14	2000
2350	1 E+11	1 E+12	1 E+13	200

Table 5.6: *Summary of radiance SNR Requirements (per FWHM)*

5.3.2.4 Dynamic Range

The dynamic range of the instrument should allow for the maximum radiance and irradiance as defined in Table 5.5 (high albedo, overhead sun, SSP …) and Table 5.6 to be measured without detector saturation. For solar irradiance and calibration measurements (for example sun over diffuser calibration) the instrument should not be saturated by looking directly into the sun via an on-board diffuser.

5.3.2.5 Straylight

The sharp increase in atmospheric photon flux of 3 orders of magnitude between 290 nm and 400 nm demands excellent straylight suppression. For any wavelength and the maximum flux given above, the contribution due to straylight from all sources (spatial, spectral, outside IFOV) shall not exceed 1 % of the signal at the wavelength in question after characterisation and adequate straylight correction.
In addition, straylight introducing spectral structures (for example ghosts) interfering with the trace gas absorption shall not exceed 0.1% of the signal at the wavelength in question after characterisation and adequate straylight correction.

5.3.2.6 Radiometric Accuracy

Relative Accuracy on Spectral Scales of Species to be detected

Experience with DOAS retrieval has shown that the relative variation in the instrument response function between adjacent pixels has to be known within 0.02% for solar irradiance and nadir radiance measurements. This includes effects like interference from diffuser, spectral structures introduced by a polarisation scrambler, variations in the quantum efficiency of adjacent pixel, detector etalons etc.

Absolute Accuracy

Other retrieved atmospheric parameters of important constituents cannot be obtained using differential methods, and are instead retrieved from the ratio of absolute numbers of earth shine radiance to solar irradiance. An important example is stratospheric ozone. This quantity will be retrieved by methods using the radiometric calibrated radiance and irradiance spectra and requires a relative to the solar irradiance radiometric accuracy of 2 – 3%.

Co-registration between the different spectral channels

The co-registration knowledge between the same spatial pixels in the different spectral groups (channels) should be 10% of a spatial pixel.

Co-registration within a spectral channel

Within any spectral group (channel), every pixel in the spectral direction shall observe the same ground scene. The image distortion shall not be more than 10% of a ground pixel.

5.3.3 Polarisation Measurement Requirements

The sections above are focussing on a spectrometer dedicated to trace gas measurements. Determining the AOT and the aerosol type over land with intensity measurements in the wavelength ranges discussed above alone is nearly impossible as it will result in very challenging radiometric calibration requirements (approx.1%) and is further complicated due to discrimination from surface albedo effects. To also address the requirement to determine AOT and aerosol type over land, it is therefore proposed to add an Aerosol Polarisation Measurement System (APMS) to the spectrometer.

As the APMS is driven by the user requirement on aerosol, it has priority A.

The requirement for the APMS are driven by the need to provide quantitative information on AOT and SSA. The requirements on the PMS are as follows (GOME-2 heritage) and based on retrieval simulations by SRON/O. Hasekamp. The APMS shall measure the three Stokes parameters I, Q and U describing polarised radiance in the wavelenght range 300 – 1000 nm with a spectral resolution starting with 2 nm in the UV (steep gradient in the degree of lin. polarisation) and ending with approx. 10 - 20 nm in the NIR (approx. linear interpolation UV –NIR). The S/N should be >500 for wavelength > 350 nm and > 100 for the UV below 350 nm. The IFOV of the PMS shall be smaller or identical compared to the main solar backscatter spectrometer (5 km x 5 km). As a goal the IFOV of the PMS shall be 2.5 km x 2.5 km. The polarisation measurements shall have the same temporal coverage as the main spectrometer, and the measurements shall be synchronised with the measurements of the main spectrometer.

5.3.4 Calibration Requirements

The retrieval of aerosol parameters, cloud cover, surface spectral reflectance and the abundances of absorbing trace gases require excellent radiometric and accurate spectral calibration of the instrument. Calibration will be performed on ground under flight-representative conditions where necessary. After launch, part of the calibration needs to be l be verified and updated with in-flight calibration, followed by regular instrument monitoring to ensure a high data quality and up-to-date knowledge of the instrument response during mission lifetime. The calibration concept is based on the heritage of SBUV, GOME (Diebel et al. 1995, SERCO 2002/2004) and SCIAMACHY (Lichtenberg et al. 2005 and references) calibration. The following is recommended to fullfill the requirements given above:

- The instrument shall be designed such that it can observe the solar spectrum via a diffuser plate and the entire optical train including the scan mirror.
- Calibration and optical monitoring activities, require the following instrument hardware: diffusers (nominal and reference), reference nadir mirror, UV enhanced white light lamp including dedicated mask hole pattern for spatial co-registration, spectral line source.
- The instrumental slit function needs to be characterised on-ground.
- This required hardware combined with dedicated measurement sequences will be used to calibrate and monitor the instrument in-flight.
- In case the trace gas spectrometer channels can not be build polarisation insensitive, the instrument shall provide means to measure the polarisation state of the incoming light as a function of wavelength. In this case the polarisation of the incoming light has to be measured parallel and perpendicular to optical plane of the spectrometer (parallel and perpendicular to the spectrometer slit).
- Long term drifts in the radiometric calibration should be minimised by an adequate in-orbit radiometric calibration using for example solar measurements via an on-board diffuser and internal calibration targets.

5.3.5 Geostationary Solar Backscatter Instrument: Notes on Feasibility

Design concepts for a solar backscatter sounder in geostationary orbit were assessed for feasibility and robustness since 1998 by several studies and groups including industry (Astrium, TPD-TNO, SIRA etc.) and agencies (DLR, ESA/EUMETSAT, NERC/UK) coming systematically to very similar conclusions that instrument concepts are mature (see for example ESA's evaluation of GeoSCIA on GeoTROPE in 2002) and feasible (several studies available), especially in the UV-Vis, due to the clear heritage of GOME, SCIAMACHY and OMI designs. This was confirmed again during the MTG-UVS evaluation, with the exception of a demanding spectrally high resolution O2-A band channel. This remaining issue is currently under study by EUMETSAT.

Obviously, the inverse square law w.r.t. the available number of photons was and is taken into account in the above mentioned studies. This is achieved by increasing the aperture (current designs have 70 mm to 140 mm apertures), by increasing the integration time (here the GEO orbit helps) and by having a high QE detectors and high throughput optical system in comparison for example to GOME-1. The use of 2-dimensional CCDs for tracegas remote sensing in the UV-Vis was recently demonstrated with OMI on AURA. This means that technology and methodology proposed to be applied in GEO is already proven in LEO by GOME-1, SCIAMACHY and OMI.

5.4 Thermal Infrared Sounding from Geostationary Orbit

5.4.1 Measurement Techniques used in the Thermal Infrared (TIR)

General
The techniques for infrared sounding of the chemical composition of the atmosphere from a geostationary orbit have been studied in the past by several groups (see references).

The main feature is that the viewing geometry is Nadir, so that vertical information has to be extracted from the physics of the problem, not from the geometry as compared to Limb geometry.

In case of infrared radiances containing molecular absorption and emission lines, the vertical information is contained both in the line profiles (Lorentzian part of the Voigt profile) which are pressure-dependent, and also in the relative intensities of molecular lines arising from energy levels with different energies. As a consequence, the spectral resolution of the infrared sounding instrument has a strong impact on the vertical resolution of the retrieved atmospheric concentration profiles.

In addition, the precision of the vertical profiles and of the height scale is strongly dependent on the absolute radiometric calibration of the infrared radiances.

Finally, the signal/noise ratio is a crucial parameter that has an important impact on the overall accuracy of retrieved concentrations and also on the vertical resolution.

In order to derive the instrument performance specifications for an infrared sounder on a geostationary platform, based on the level 2 requirements given in the WP2100 report, we have used the following approach.

For the radiative transfer part of the problem, we have used the results of a study carried out in a team with scientists from LISA, CNES and IMK/FZK Karlsruhe, where the impact of different instrument parameters (spectral resolution, signal/noise ratio) on the precision of retrieved atmospheric concentration profiles was investigated, using the well known KOPRA code (that is validated and used also for the MIPAS project). Due to the highly nonlinear nature of the problem, this approach is considered to be the most realistic one. Note that one can also study the "information content" of the data (as in the EUMETSAT MTG document by *Clerbaux et al.*, see references) but this approach does not directly provide the instrument specifications as a function of the level 2 data requirements.

The temporal requirements of the level 2 data have not been taken into account for the determination of instrument specifications because the specifications for the signal/noise ratio and for the radiometric calibration are independent of the temporal requirements of WP2100 (see the scheme below). However the values for signal/noise ratio and for the radiometric calibration must be seen in the context of the temporal requirement of WP2100.

Instruments used in the thermal infrared (TIR)
For infrared sensing of the atmosphere there are two types of instruments that can be used: dispersive (grating or prism) spectrometers or Fourier transform interferometers. For the following, no special instrument assumptions have been made, except for the spectral resolution which is defined as the Full-Width at Half-Maximum of the instrumental line shape, where a sinc (=sinx/x) function was assumed as instrumental line shape.

Atmospheric species absorbing in the thermal infrared (TIR)
Of the atmospheric molecules appearing in the tables of WP2100, the following have absorption or emission lines in the infrared (see

Figure 5.2); these are H_2O, CO_2, O_3, N_2O, CO, CH_4, NO, NO_2, HNO_3, OCS, CFC-11, CFC-12, HCFC-22, ClO, SF_6, HCl, BrO, $ClONO_2$, HBr, $BrONO_2$, CH_3Cl, CH_3Br, SO_2 (enhanced), CH_2O, N_2O_5, PAN, CH_3COCH_3, and C_2H_6 [Rothman et al.,, 2005].

However, several of them (BrO, HBr, $BrONO_2$, CH_3Cl, CH_3Br, CH_2O, PAN, CH_3COCH_3, C_2H_6) have not been observed in the infrared from satellites, due to missing spectroscopic parameters, or insufficient signal/noise, spectral resolution, wavelength coverage or observation geometry (often a combination of some of these reasons).

Of those, the species relevant for B1-S, B2-S and B3-S are: O_3, H_2O, NO_2, CO, SO_2, CH_2O, HNO_3, N_2O_5 (night), PAN, and Org. Nitrates.

As will be shown in the following, the instrument requirements in this Work Package are derived from the level 2 data requirements for these species. In addition, an independent requirement exists on CO_2 that translates into a requirement on vertical temperature profiles with the appropriate resolution and accuracy. However, it is projected that it will be possible to obtain accurate and suitable vertical temperature profiles from meteorological data centres within the time frame of a few years [Peuch 2005].

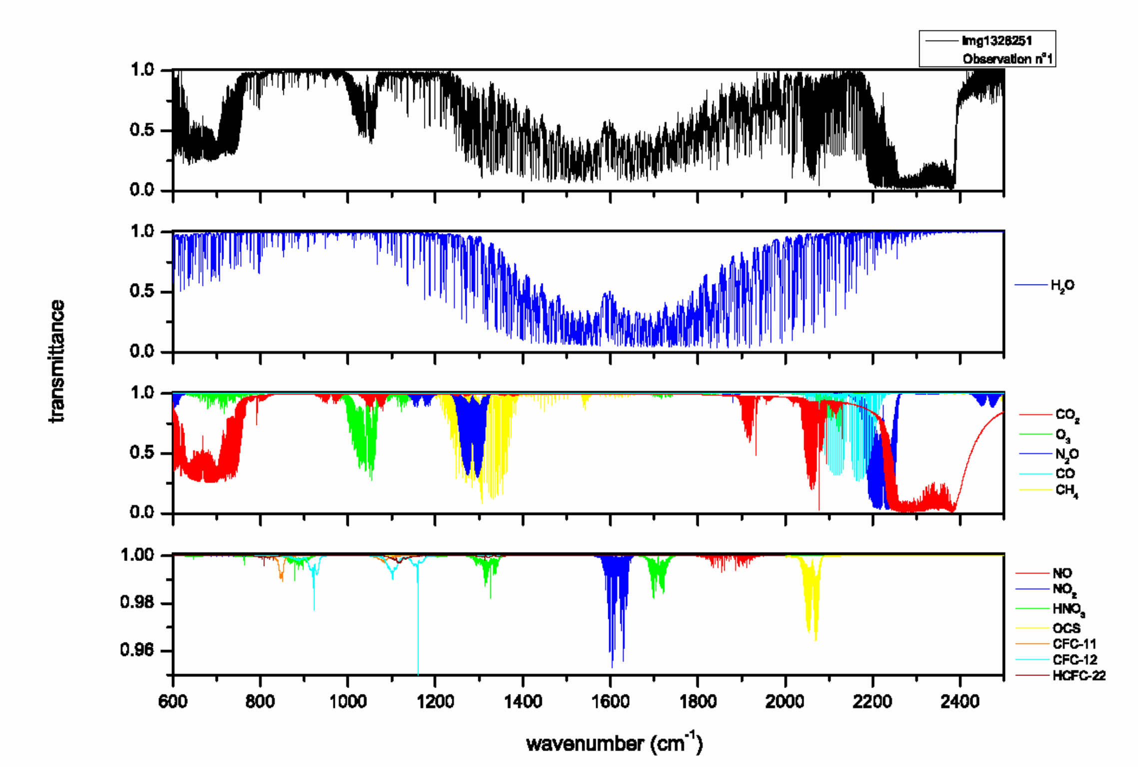

Figure 5.2. *Infrared atmospheric spectra in Nadir geometry (from Clerbaux et al. 2003a)*

The different trace gases absorb in different spectral region, so that in addition to the requirement on spectral resolution (for the vertical resolution, see above), requirements on spectral coverage will arise. The main advantages of using thermal infrared (TIR) observations are:

- In extension to instruments using solar backscattered light, TIR measurements are available during day and night.
- For species that are observed in the UV/VIS (O_3) and SWIR (CO, H_2O, CH_4, N_2O) TIR observations provide significant additional information on vertical profiles.

- A number of important atmospheric species can only be measured using TIR instruments: PAN, C_2H_6, N_2O_5, HNO_3.

5.4.2 TIR Instrument: Observations Modes

In addition to the nominal viewing mode (Earth), the TIR instrument needs two additional modes for in-orbit radiometric calibration: to on-board blackbody source(s) – possibly even two – and to cold space. Also the instrument has to be protected against direct light from the sun that would have strong impact on thermal and radiometric parameters.

5.4.3 TIR Instrument: Spectral Requirements

5.4.3.1 Infrared absorbing species and spectral coverage of the TIR instrument

As already shown in Figure 5.4**,** every molecule absorbs and/or emits at different characteristic wavelengths in the infrared. This leads naturally to requirements on wavenumber coverage (the wavenumber is defined as the inverse of the wavelength in cm).

Wavenumber Min	Max]	Product	Priority
[cm-1]	[cm-1		
720	800	CO_2/T	B
800	**900**	**HNO_3, C_2H_6**	**A**
900	**1200**	**O_3 and PAN**	**A**
1200	**1300**	**N_2O_5**	**A**
1200	1400	H_2O	B
1300	1400	SO_2	C
1580	1670	NO_2	C
1700	1800	CH_2O (and PAN)	C
2100	**2200**	**CO**	**A**
2300	2600	CO_2/T	B

Table 5.7: *Summary of Spectral Coverage Requirements. Priority A: Unique contribution of IR (HNO_3, PAN, N_2O_5) or important synergism with solar backscatter (O_3, CO). Priority B: Covered by MTG-IRS and available in the future from other services: H_2O, CO_2/T. Priority C: Covered by solar backscatter instrument*

Note to Table 5.7:
If for the TIR instrument one focuses on class “A” priorities, a significantly reduced spectral coverage is obtained (800-1300 cm^{-1} and 2100-2200 cm^{-1}). The reason is that vertical profiles of temperature (CO_2/T) and humidity with sufficient accuracy should be available from meteorological services (therefore priority “B”), and that species with weak infrared absorptions (SO_2, NO_2, CH_2O) can be easily observed by a solar backscatter (UV/VIS/SWIR) instrument (therefore leading to priority “C” in the TIR table). This means that a combined TIR – UV/VIS/SWIR mission leads to significantly reduced requirements on the TIR instrument as far as spectral coverage is concerned.

5.4.3.2 Vertical resolution requirements and spectral resolution of the TIR instrument

As said before, the line widths of atmospheric molecules in the thermal infrared (TIR) are pressure-dependent and provide therefore information on the vertical distribution of these species. The molecular line widths are typically around 0.15-0.40 cm^{-1} (full-width at half maximum, FWHM) in the lowest atmospheric layers and decrease with increasing altitude.
The impact of spectral resolution on the accuracy of trace gas concentrations and vertical resolutions was investigated for three different resolutions (0.125, 0.25 and 0.5 cm^{-1}) and for different values of the signal/noise ratio. Calculations were carried out only for H_2O, O_3, and CO. For the other relevant species in Tables B1-S, B2-S and B3-S (i.e. NO_2, SO_2, CH_2O, HNO_3, N_2O_5 (night), PAN, and Org.

Nitrates) it was found that only tropospheric columns are feasible which depend much less on spectral resolution and are therefore not a driver for such an instrument specification.
The influence of thermal contrast (temperature difference between surface and the lowest atmospheric layers) is of course very significant. For example, for ozone, thermal contrast leads to strong variations of the retrieval error for the lowest layer (in the retrievals fixed to 0-2 km, see the following table 8).

T_{surf} (K)	Error PBL (0-2 km) in %	Error LT (2-	Error UT (7-	Mean vertical resol. (km)
270	***8.6***	***7.5***	***4.8***	***6.3***
275	***18.8***	***11.4***	***5.5***	***5.7***
280	***52.0***	***23.6***	***12.3***	***6.3***
288	***29.4***	***16.2***	***14.2***	***5.5***
290	***26.2***	***14.5***	***13.2***	***5.6***
300	***19.5***	***11.9***	***12.2***	***6.1***

Table 5.8: *Impact of thermal contrast on ozone error (spectral resolution 0.25 cm^{-1}, altitude grid and vertical temperature profile used).*

The requirements on vertical resolution from Tables B1-S, B2-S and B3-S vary between 1 km and tropospheric columns. Since in the simulated TIR retrievals the **degrees of freedom in the troposphere (0-15 km) were set to 3 for O_3 and CO** and at 7 for H_2O (using first-order Tikhonov constraint), the impact of spectral resolution on vertical resolution seems to be relatively small. However, its strong impact is clearly visible in the accuracies of the retrieved concentrations. For instance, in the Lower Troposphere (LT) the mean vertical resolution is 5-6 km for O_3 and CO for all values of spectral resolution, but the accuracy decreases dramatically when reducing the spectral resolution. Because the requirements for signal/noise and spectral resolution are related due to the non-linear nature of the retrieval process in the TIR region, it is impossible to derive an absolute requirement for spectral resolution only, without taking into account also the signal/noise ratio. For instance, if one takes the requirement for O_3 from Tables B1-S, B2-S and B3-S (i.e. 10% uncertainty in the PBL) it is clear that this can be only be achieved with

- a resolution of 0.25 cm^{-1} and a signal/noise ratio higher than 4800, or
- with a resolution of 0.125 cm^{-1} and a signal/noise ratio higher than 2400.

For CO, the requirement from Tables B1-S, B2-S and B3-S is 20% in the PBL. This can be achieved

- with a spectral resolution of 0.25 cm^{-1} and a signal/noise ratio of about 450, or
- with a spectral resolution of 0.125 cm^{-1} and a signal/noise ratio of about 225.

For NO_2, the requirement on 20% of the tropospheric column is very difficult to achieve, because of strong overlap of H_2O absorption (see Figure 5.4). It is clear however, that the highest spectral resolution (0.125 cm^{-1} or better) and signal/noise ratio (above 2500) are required. (See *Wetzel et al., 1995* and *Clerbaux et al., 2003*).

Although no particular instrument design can be derived from the requirements given above it is important to stress that the influence of the knowledge of the instrumental line shape (ILS) on the error budget was neglected. This assumption therefore translates into a calibration requirement, see below (section 5.4.5).

5.4.4 TIR Instrument: Radiometric Requirements

The radiometric requirements can be separated into requirements on the signal/noise ratio (see above) and requirements on the radiometric accuracy (with an impact on radiometric calibration). The latter will be dealt with in Section 5.3.2.5 (Calibration Requirements).

5.4.4.1 Accuracy of trace gas concentrations - signal/noise ratio of the TIR instrument

As far as the signal/noise ratio is concerned, the tables in Section 5.4.3 (Spectral Requirements) show that the signal/noise ratio and the spectral resolution are related. If we use a spectral resolution of 0.125 cm^{-1}, the following table is obtained in order to fulfil the requirements of Tables B1-S, B2-S and B3-S (we have added C_2H_6 as a typical VOC):

spectral range (cm^{-1})	signal/noise ratio	spectral resolution (cm^{-1})	target species
800-850	1200	0.125	C_2H_6
850-900	1000	0.125	HNO_3
900-1200	2400	0.125	O_3, PAN
1200-1400	2400	0.125	H_2O, SO_2, N_2O_5(night)
1580-1670	>2500	<0.125	NO_2
1700-1800	1000	0.125	H_2CO, PAN
2100-2200	450	0.25	CO

Table 5.9: *Signal/noise ratio requirements for a TIR instrument addressing B1-B3. Note: Not included here are signal/noise ratio requirements for CO_2 (necessary for temperature profile retrieval), since accurate vertical temperature profiles should be available from other sources (meteorological services, see below).*

Combining TIR with solar backscatter leads to a significant relaxation w.r.t. spectral range and SNR.

spectral range (cm^{-1})	signal/noise ratio	spectral resolution (cm^{-1})	target species
800-900	1200	0.125	HNO_3, C_2H_6
900-1200	1200	0.125	O_3, PAN
1200-1300	1200	0.125	H_2O, N_2O_5(night)
2100-2200	450	0.25	CO

Table 5.10: *Signal/noise ratio requirements for a TIR instrument combined with a UV/VIS instrument (see Section 5.3); the relaxed S/N has been applied for the O_3 region.*

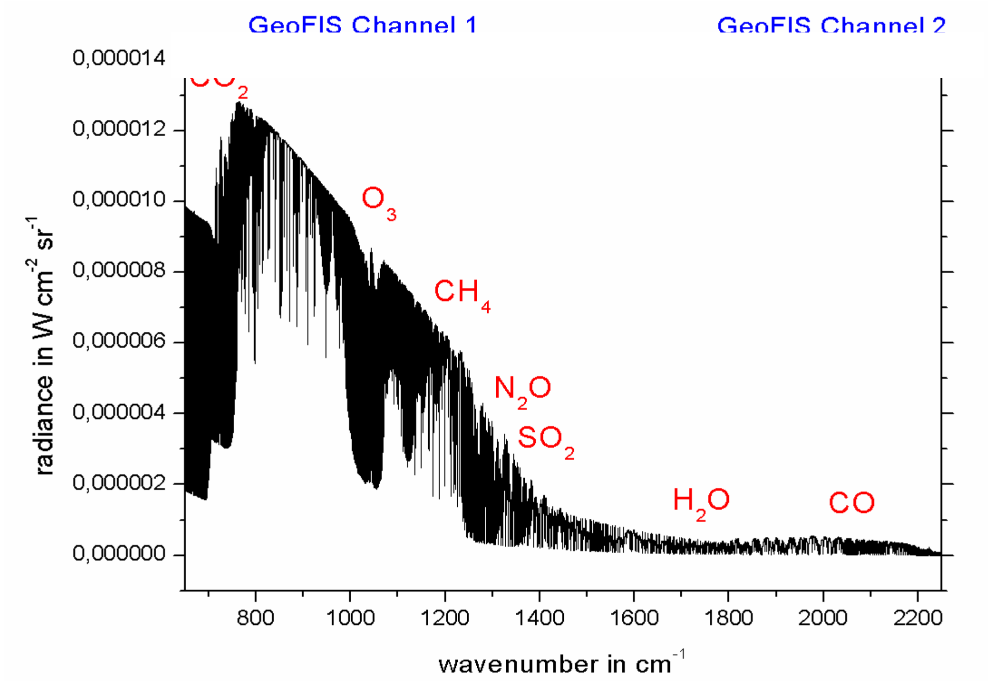

Figure 5.5 *Reference spectrum used for the TIR requirements (in W cm^{-2} sr^{-1} cm^{-1}).*

Note: These signal/noise values can be translated into Noise-Equivalent Spectral Radiances (NESR) using the reference spectrum. For example, NESR is 2.525 - 3.35 nW / (cm^2 sr cm^{-1}) in the O_3 region (900-1100 cm^{-1}) and 0.525-0.55 nW / (cm^2 sr cm^{-1}) in the CO region (2100-2200 cm^{-1}).

5.4.4.2 Radiometric accuracy

Based upon previous studies for TIR sounders in GEO and also in LEO orbits, a radiometric accuracy of 0.5 K is considered to be adequate to achieve the vertical resolution and accuracies required from the Data Requirement Tables B1-S, B2-S and B3-S.

5.4.5 Calibration Requirements for the TIR Instrument

To illustrate the approach followed here, the calibration allocation tree from the GIFTS study is shown below

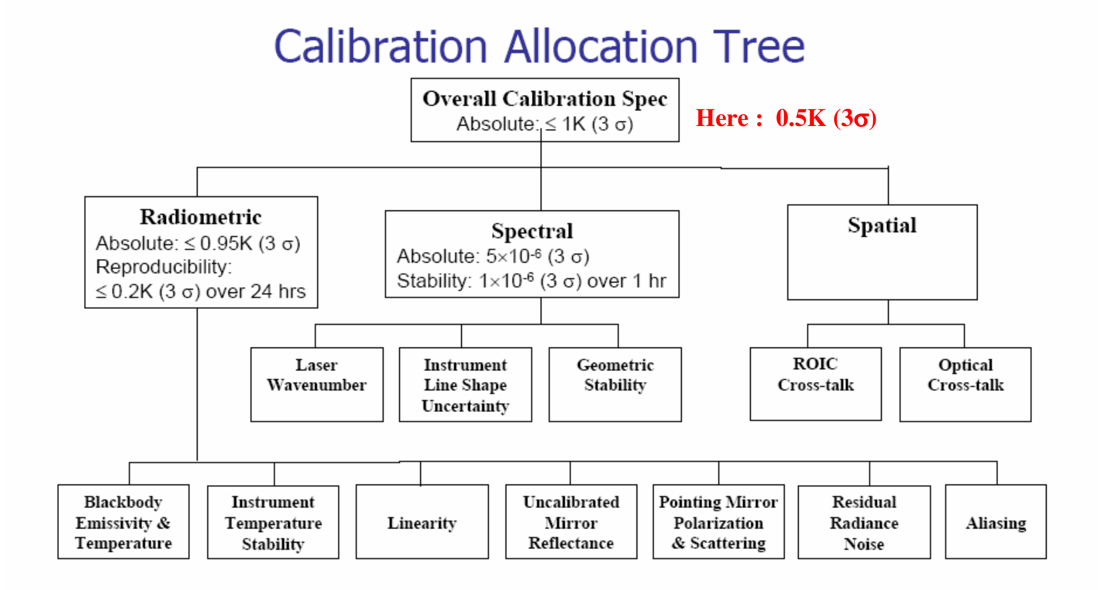

Figure 5.6. The calibration allocation tree from the GIFTS study

5.4.5.1 Radiometric calibration of the TIR instrument

The radiometric calibration can be separated into absolute calibration and reproducibility. For example, if we use a factor of two (overall requirement for radiometric accuracy 0.5 K in this study compared to 1 K (3σ)) for GIFTS), the allocation is ≤ 0.47 K (3σ) for absolute calibration and ≤ 0.1 K (3σ) for reproducibility. The radiometric calibration can be broken down into calibration of blackbody emissivity and temperature, instrument temperature stability, linearity, mirror properties, residual radiance noise and aliasing (for a Fourier transform spectrometer, for a dispersive spectrometer this corresponds roughly to straylight or light from higher orders for a grating instrument).

5.4.5.2 Spectral calibration of the TIR instrument

The spectral calibration comprises absolute calibration, requirement 2E-06 (3σ), and stability, requirement ≤ 1E-06 (3σ). The idea is to constrain spectral calibration so that it does not contribute significantly to the error budget. Note that in the KOPRA calculations shown before, the error due to the knowledge of the instrumental line shape (ILS) was assumed to be negligible. Characterisation of the ILS function is therefore an important requirement.

5.4.5.3 Spatial calibration

This is related to Pointing Stability and Knowledge that have been dealt with in Section 5.**Error! Reference source not found.**.

5.4.6 Conclusions on TIR Geostationary Instrument Specifications

The specifications for the TIR Geostationary instrument have been derived from the requirements presented in CAPACITY Task 2 (see tables of WP 2100). For this purpose, radiative transfer calculations were carried out using the KOPRA code developed at IMK/FZK in frame of the MIPAS project. Synthetic retrievals were performed using the associated inversion code of KOPRA, with 3 degrees of freedom (first-order Tikhonov constraint) for O_3 and CO in the troposphere.
It is shown that a combined mission with both TIR and UV/VIS.SWIR instruments leads to significantly reduced requirements concerning the spectral coverage for the TIR instrument.

For the vertical profiles of temperature and humidity, it is anticipated that these will be available from meteorological services. The influence of the knowledge of vertical temperature profiles was studied in detail for O_3 and CO. An uncertainty of 0.5-1.0 K, together with appropriate microwindow selection, will be sufficient in order to reduce the impact of the knowledge of vertical temperature profiles to less than the uncertainty due to signal/noise ratio. Such a knowledge on T profiles is projected to be feasible within the next years (Peuch, 2005). Therefore, no additional requirements on the accuracy of temperature profile retrieval (using CO_2 bands) or of H_2O profile knowledge have been formulated.

5.4.7 Geostationary Infrared Instrument: Note on Feasibility Study

Starting in fall 2003, a study was performed by the CNES PASO group in Toulouse (France), in order to evaluate the feasibility of a geostationary infrared instrument. This study was initiated after the proposal of the Geostationary Fourier Imaging Spectrometer (GeoFIS, see Flaud et al., 2004) as part of the GeoTroPE mission (see Burrows et al., 2004). Since the results of this study are also of interest for the CAPACITY project, we think it is appropriate to provide a few details of this study. More information can be obtained from the reference documents that are available upon request to CNES.

Two sets of instrument specifications were provided as input to the CNES team: “goal” and “threshold” specifications. They correspond to the two sets of specifications provided above, in particular the “threshold” specifications are covering a reduced spectral range because a simultaneous UV/VIS instrument is supposed.

In addition to the instruments, different launchers, platforms, and also the influence of clouds have been studied in the frame of the CNES PASO study.

Two different instrument types have been studied by CNES: a diffractive instrument and a Fourier-transform spectrometer. However, the dimensions of the diffractive instrument are such that the CNES engineers consider that this instrument is not feasible. Therefore, the design study of a Fourier-transform spectrometer was followed. Within this architecture, different detector arrays and optical arrangements were investigated (e.g. matrices of 128×128 pixels or of 320×255 pixels), and several optical parameters were varied (pupil diameter varying from 5 cm to 15 cm, use of a telescope, number of spectral channels, integration time etc.). Also thermal stability and vibrational analysis have been carried out.

In conclusion (see the most recent document) the CNES PASO engineers have judged the TIR instrument as feasible. Although several items have been identified as being difficult from the technological point of view, the feasibility of the thermal infrared instrument in GEO has not been jeopardized.

From the CNES study, the instrument dimensions are (estimated) 1,00 m x 0,56 m x 0,35 m, and the mass to 100-150 kg.

5.5 Expected Performance and Comparison to User Requirements

5.5.1 Aerosol

O.Hasekamp investigated the expected performance of a polarisation measurement system in geostationary orbit by using polarimeteric and multi-angular viewing (see Annex B (?)), in comparison to pure single angle intensity measurements, assuming a bi-modal aerosol model (here industrial aerosol) with 5 free parameters per mode: effective radius, effective variance, aerosol column, real/imaginary part of refractive index.

Measurements of I and Q component in the spectral range 350 to 1000 nm results in error on AOT well below (@ 550 nm) the requirement (0.05).Measurements of I, Q and U further reduces the error on AOT (roughly factor 2), resulting in AOT @ 350 nm also be within 0.05. The degree of freedom is between 6 and 7, which means that there is the potential to discriminate the fine and the coarse mode.

In addition, the single scattering albedo (SSA) at 350 nm can be determined with an error of 0.004 to 0.005.

The combination of AOT and SSA will allow to derive information on the aerosol type.In summary, the AOT requirement can be addressed with a polarisation measurement system in geostationary orbit, yielding data with hourly temporal sampling and 5 km horizontal resolution.

5.5.2 Trace Gases from Solar Backscatter

Based on the instrument specification and retrieval simulations the performance of the solar backscatter sensor w.r.t. the L2 requirements was assessed. The retrieval simulations were performed within the EUMETSAT CUVVISI study [CUVVISI]. The relevant report is available from www.eumetsat.de. Also error budgets are provided there [CUVVISI], based on literature survey and instrument studies performed during the last years (Kerridge et al. 2002, O'Brien et al. 2003, Bovensmann et al. 2004). In addition, results from real retrieval based on GOME and SCIAMACHY data including validation results were used to check that the expected performance is in line with the already demonstrated performance of instruments in LEO.

In Table 5.12 the expected performance for a solar backscatter instrument (row "solar") in geostationary orbit is compared to the CAPACITY user requirements.

5.5.3 Trace Gases from TIR

Based on the instrument specification and retrieval simulations the performance of the TIR sensor w.r.t. the L2 requirements was assessed. The retrieval simulations were performed by the team at IMK-FZK (Karlsruhe) in collaboration with LISA (Créteil) within the CNES-PASO study on the GeoFIS instrument designed and performance. The details of this study can be obtained upon request to the CNES. Note that a similar retrieval study was performed by *Clerbaux et al.* for EUMETSAT leading to the same results.

In Table 5.12 the expected performance for a TIR instrument (row "TIR") in geostationary orbit is compared to the CAPACITY user requirements.

5.5.4 Combined Retrieval

The potential to improve the accuracy of tracegas retrieval by combined solar backscatter and IR sounding was assessed by combined retrieval simulations. A two-step retrieval was used. Starting point is the IR retrieval. The output from the IR retrieval is then used as a-priori input to the solar backscatter retrieval. The results for O_3 and CO are summarised in the table below and are compared to the user requirements in Table 5.12 (row "combined".

The combination of TIR and solar backscatter results in a significant improvement in the tropospheric sensitivity. Especially in the lower troposphere (0-2 km) a significantly enhanced precision is seen, directly addressing the user needs on quantitative PBL information. The results are in line with earlier published results [Bovensmann et al. 2002].

Species		**Vertical layers** 0–2 km	2-7 km	7-12 km
O_3	**combined**	**5 %**	**< 5 %**	**< 5 %**
	TIR	15 %	10 %	10 %
	Solar Backscatter		Column 10 - 20%	
CO	**combined**	**10 %**	**< 10 %**	**< 10 %**
	TIR	20 %	10%	10 %
	Solar Backscatter		Column 10 - 20%	

Table 5.11: *Expected performance of the combined TIR- solar backscatter retrieval.*

Parameter		**Uncertainty**	**Horizontal Resolution (@Europe) [km]**	**Vertical Resolution Troposphere [km]**	**Revisit Time [hours]**
O_3	**Req.**	**10 – 25 %**	**5 – 20**	**1-3 - TrC**	**0.5 - 2**
	Solar	10 – 20%	5-10	TrC	1
	TIR	10 – 20 %	15 – 25	5 – 6	1
	Comb.*	< 10	15 – 25	2/5-6	1
NO_2	**Req.**	**10 – 30 %**	**5 – 20**	**1-3 - TrC**	**0.5 – 2**
	Solar	20 - 30 %	5-10	TrC	1
CO	**Req.**	**20 – 25 %**	**5 – 20**	**1-3 - TrC**	**0.5 – 2**
	Solar	10 – 20 %	5-10	TrC	1
	TIR	10 –20 %	15 – 25	5-6	1
	Comb.*	< 10 %	15 – 25	2/5-6	1
SO_2	**Req.**	**20- 50%**	**5 – 20**	**1-3 - TrC**	**0.5 – 2**
	Solar	30-40 %	5-10	TrC	1
HCHO	**Req.**	**20-50%**	**5 – 20**	**1-3 - TrC**	**0.5 – 2**
	Solar	30-40 %	5-10	TrC	1
Aerosol Optical Depth	**Req.**	**0.05**	**5 – 20**	**-**	**0.5 – 2**
	Solar	< 0.05	5-10	-	1
Aerosol Type	**Req.**	**< 10% mis-assignments**	**5 – 20**	**-**	**0.5 – 2**
	Solar	TBD	5-10	-	1
H_2O	**Req.**	**10 – 20 %**	**5 – 20**	**1-3- TrC**	**0.5 – 2**
	Solar	10 %	5-10	TrC	1
	TIR	1-2%	15 – 25	2 - 3	1
HNO_3	**Req.**	**20 %**	**5 – 20**	**1-3 – TrC**	**0.5 – 2**
	TIR	(Note 1)	15 – 25	TrC	1
N_2O_5 (night)	**Req.**	**20 – 50%**	**5 – 20**	**1-3 - TrC**	**0.5 – 2**
	TIR	(Note 1)	15 – 25	TrC	1
PAN	**Req.**	**20 %**	**5 – 20**	**1-3 - TrC**	**0.5 - 2**
	TIR	30%	15 – 25	TrC	1
Organic Nitrates (B3-S only)	**Req.**	**30 %**	**5 – 20**	**PBL only**	**0.5 - 2**
	TIR	(Note 1)	15 – 25	TrC	1

Table 5.12: *Comparison of expected performance of GEO instrumentation and CAPACITY user requirements (yellow: meets threshold, green: (nearly) meets goal).*enhanced sensitivity to 0-2 km layer. Note 1: Uncertainties for HNO_3, N_2O_5 (night) and Organic Nitrates cannot be established without further studies.*

5.6 Conclusions

A solar backscatter instrument in geostationary orbit was specified to provide during daylight total and tropospheric column information on O_3, NO_2, SO_2, HCHO, H_2O and CO as well as AOT, including the lowest troposphere with one hour sampling and at 5 km x 5 km horizontal resolution (SSP).
A thermal IR instrument in geostationary orbit (15 km x 15 km horizontal resolution, 1 hour temporal sampling) can provide height information in the troposphere on O_3, CO and H_2O during day and night.In addition, thermal IR has the potential to provide column of HNO_3, PAN, N_2O_5 (night), and Organic Nitrates.
The combination of Solar Backscatter and IR will result in improved height resolved information weighted towards the including the lowest troposphere for O_3 and CO. Assuming that H_2O as well as CO_2/T are covered by MTG-IRS, two mission scenarios for the geostationary componennt of an operational atmospheric monitoring system can be identified:

A) A combined solar backscatter and TIR sounding mission addressing B1-B3 requirements

- Combined Solar Backscatter – TIR sounding: height resolved O_3 and CO with enhanced PBL sensitivity,
- Solar backscatter will provide total and tropospheric columns of NO_2, SO_2, HCHO as well as data on aerosol (AOT etc.)
- TIR will in addition provide HNO_3, PAN, N_2O_5 (night) and Organic Nitrates

B) A solar backscatter sounding mission addressing B1 requirements

- Solar Backscatter provides total and tropospheric column information on O_3, NO_2, CO, SO_2, and HCHO as well as AOT, including the lowest troposphere (at one hour sampling and at 5 km x 5 km (SSP)).
- Addition of H_2O can address B3
- No data on HNO_3, PAN, N_2O_5 and Organic Nitrates
- No nighttime coverage
- No height resolved information on O_3 and CO in the troposphere.

The methodology to derive tropospheric trace gas distributions from space is already demonstrated by LEO instruments.

The table below summarises the contribution of a geostationary component of an operational atmospheric chemistry monitoring system to the CAPACITY application areas in comparison to METOP/NPOESS.

Application	User	Cat.	Metop/NPOESS Non-Compliance w.r.t. CAPACITY	added value of GEO European AQ mission
Ozone/UV	A1S	protocol		
	A2S	operational	absence of stratospheric profile data	for UV forecast Europe: O3, aerosol, revisit time 1 h, horizontal resolution < 20 km
	A3S	assessement	absence of stratospheric profile data	
Pollution monitoringand AQ forecast	B1S	protocol	revisit time < 2h, horizontal resoluton < 20 km, GOME-2/IASI will give survey	trace gases, aerosol, revisit time 1 h, horizontal resolution 10 - 25 km
	B2S	operational	revisit time < 2h, horizontal resoluton < 20 km,	trace gases, aerosol, revisit time 1 h, horizontal resolution 10 - 25 km
	B3S	assessement	revisit time < 2h, horizontal resoluton < , 20 km	trace gases, aerosol, revisit time 1 h, horizontal resolution 10 - 25 km
Climate	C1S	protocol	Lack of boundary layer sensitivity CH4, CO2, CO, aerosol	CO, aerosol over Europe
	C2S	operational	absence of profiles from tropopause upwards	H2O, O3, aerosol over Europe
	C3S	assessement	absence of profiles from tropopause upwards	
			Major	Major
			Significant	Significant
			Minor	Minor

Figure 5.7. Contribution of the geostationary component of an operational atmospheric chemistry monitoring system on the CAPACITY application areas in comparison to Metop/NPOESS.

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6 Instrument Performance and Requirements for LEO

6.1 Introduction

Measurement techniques were reviewed to identify the contributions which each could potentially make to monitoring atmospheric composition from low earth orbit, focusing specifically on the value which each would add to the planned operational observing system constituted by MetOp/NPOESS. To inform this review, quantitative comparisons against observational requirements were performed for each application using performance estimates from retrieval simulations for instrument specifications which were made available to the study from other projects. Findings were then drawn for each application in regard to the overall value which each measurement technique could add to the planned operational system.

6.2 Background

This assessment of low-Earth orbiting (LEO) mission capabilities is intended to identify and collate information on instruments for a potential future LEO mission. A number of the instrument concepts under consideration have been defined in previous studies for and Explorer-class mission including "Definition of Mission Objectives and Observational Requirements for an Atmospheric Chemistry Explorer Mission" (ESA Contract 13048/98/NL/GD), also referred to as the ACOR Study, and the "Report for Assessment of the ACECHEM Candidate Earth Explorer Core Mission" (ESA SP-1257(4)). In the ACOR study, the techniques which were found to be best-suited to observing each constituent in a given height-range, as defined in Table 6.1, are summarised in Table 6.2. Several further possibilities were speculated upon (identified in the Table by italics), but were beyond the scope of the study to examine quantitatively. Following the approach adopted for existing and planned missions in WP2200, the performance of the new instrument concepts was assessed against the data requirements set in WP2100.

Domain name	Altitude range (km)
Lower Troposphere (LT)	0-8 *
Upper Troposphere (UT)	8 – TP
Lower Stratosphere (LS)	TP – 24
Middle Stratosphere (MS)	24-36
Upper Strat. and Mesosphere (US + M)	36-80

* UT at latitudes above 70^0 latitude starts at 5 km. TP = tropopause

Table 6.1. The atmospheric domains used in the ACOR study

	LT	UT	LS	MS/US
Limb				
UV	-	-	-	BrO, OClO
VIS	-	-	NO_2, (O_3), *aerosol*	(NO_2), (O_3)
NIR	-	-	*aerosol*	
MIR	-	(H_2O), (O_3), HNO_3, C_2H_2, C_2H_6, PAN, CH_3COCH_3, *aerosol*	H_2O, O_3, HNO_3, N_2O, CH_4, CFCs, HCFCs, aerosol, T	As LS + NO_2, N_2O_5, $ClONO_2$
FIR	-	-	OH	OH, HO_2,H_2O_2
Sub-MM	-	-	ClO, HCl, HOCl, CH_3Cl, (BrO), HBr, CH_3Br	ClO, HCl, HOCl, (BrO), HBr, NO
MM	-	H_2O, O_3, CO	H2O, O3, CO, HNO_3, N_2O	As LS
Nadir				
UV	O_3, H_2CO(T), SO_2(T)	(O_3), H_2CO(T), SO_2(T)	(O_3), SO_2(T)	(O_3)
VIS	NO_2(T)	NO_2(T)	NO_2(T)	-
NIR	Aerosol, H_2O, CO, *HCs*	Aerosol, (H_2O), (CO), *HCs*	-	-
MIR	T, H_2O, CO, *HCs*	T, (H_2O), (CO), *HCs*	-	-
MM	(H_2O)	(H_2O)	-	-

Brackets indicate that measurements would be made by this technique of this species in this height range, but would be less valuable than other measurements. (T) signifies total column measurement.

Table 6.2: Principal Species Assignment in Different Height Ranges as derived in the ACOR study.

6.3 Descriptions and Detailed Assessment of New Instrument Concepts

A number of new instrument concepts under development were available to be assessed in detail. The performance of the following were considered :

MASTER : A millimetre-wave/ sub-millimetre wave limb-sounder
AMIPAS : An infrared FTS limb-sounder
Limb UV-VIS-NIR Spectrometer (SCIAMACHY derived): A limb-UV/VIS/NIR grating spectrometer
Multi-angle Polarimeter : A multi-view, nadir and off-nadir, polarisation-sensitive UV-VIS instrument targeting aerosol
Nadir-UV-VIS Spectrometer (OMI derived) : A multi-view, nadir and off-nadir, UV-VIS instrument targeting ozone (two closely related options, one of which includes polarisation measurements are included)
Nadir UV-VIS-NIR-SWIR 2D Imaging Spectrometer (OMI derived): A 2D grating concept making near-infrared measurements
Nadir-SWIR Spectrometer (OMI derived): A nadir near-infrared nadir viewing grating spectrometer
Nadir-SWIR (SCIAMACHY derived) : A new version of the SCIAMACHY instrument (UV-VIS-NIR-SWIR nadir viewing grating spectrometer) which avoids ice contamination

Basic descriptions and instrument specifications are given in the Technical Note on this work package (WP3200). The detailed analysis employed for the new sensors followed the methodology of the "Assessment of Existing and Planned Atmospheric Sounding Missions and Networks" (WP2200). Performance data was collated and comparisons against requirements presented in table form. The detail of the analysis, including a full set of tables, is presented in the Technical Note on this work package (WP3200)

6.4 Overall Assessment of Relevant Measurement Techniques

The overall assessment of measurement techniques drew on the detailed quantitative analyses of new sensors as well as existing and planned missions performed previosuly in WP2200. The general characteristics of other new sensors were also taken into consideration if performance estimates were not available.

6.4.1 UV/VIS & IR Solar Occultation

Stratospheric measurements by ir and uv/vis solar occultation instruments offer intrinsically high precision, vertical resolution and long-term stability and have arguably provided the most valuable satellite contributions (e.g. SAGE-II, HALOE) to the quantification and attribution of height-resolved, longterm trends in ozone and other stratospheric constituents. Solar occultation data have also been assimilated into chemical transport models for research purposes although, due to the very sparse geographical sampling of O_3 and H_2O by comparison to other data sources, their impact is not sufficient to justify assimilation into forecast models by the operational centres.

There are currently no planned missions of this kind to follow ACE and MAESTRO on SCISAT, and these are unlikely to function beyond 2010. Instruments of this kind on a Sentinel mission could therefore be of great value to the "scientific assessment" user categories in the ozone/uv and climate applications, in spite of their gross non-compliance on horizontal sampling.

6.4.2 Lidar / DIAL

The lidars launched on CALIPSO (2005), ADM-Aeolus (2007) and EarthCARE (2012) will profile tropospheric aerosol at comparatively high vertical resolution along sub-satellite tracks. The utility of such measurements for pollution monitoring, air quality forecasting and other operational applications will be evaluated through assimilation by ECMWF, national met services and research institutes during the coming decade.

A lidar flying in parallel to EarthCARE could double the geographical sampling of cloud-free scenes per day. If a sun-synchronous orbit with distinctly different equator crossing time was selected, this could further increase value for air quality forecasting.

An aerosol lidar deployed in a dedicated Sentinel mission would therefore enable requirements for tropospheric aerosol profile data in all user categories and application areas to be better served, in spite of being grossly non-compliant on horizontal sampling.

Should ADM-Aeolus wind measurements be demonstrated to have a significant positive benefit to NWP, Eumetsat might wish to consider a Doppler wind lidar for the post-EPS system, which would also provide aerosol profile data.

The value of the DIAL technique could potentially be to sound tropospheric trace gases with higher vertical resolution than can be attained by passive techniques, and specifically to resolve the boundary layer. The wavelength range accessible to DIAL is governed primarily by (Rayleigh and) aerosol scattering efficiency, which effectively means the near-UV to near-IR, which excludes almost all fundamental vibration-rotation bands. With the exception of ozone, for which differential structure in the Huggins-bands (arising from vibrational structure in an electronic transition) can be exploited, the only differential structure available is therefore from transitions in comparatively weak vibration-rotation combination and overtone bands. Some possible candidates are therefore H_2O, CO_2 and possibly CH_4 . Cleanly resolving the boundary layer from the free troposphere would be a major advance for either CO_2 or CH_4 .

DIAL instruments on the ground and aircraft have yielded high-quality profiles on O_3 and H_2O. DIAL concepts have also been proposed for space and the WALES concept for H_2O was studied to Phase A by ESA. However, none has so far been selected for implementation by the Space Agencies. Value added to passive FTIR nadir-sounding seems not to be clear-cut, since this would be confined mainly to the lower troposphere, where H_2O can be retrieved from the FTIR with quite high (~1km) vertical resolution, and also to the sub-satellite track. Technical risk (and therefore cost) currently place this outside scope for consideration for a Sentinel mission.

6.4.3 Multi-angle Polarimeter

Downward-viewing vis/ir imagers are integral to the MetOp/NPOESS operational observing system and will also provide cloud and aerosol information from research satellites planned in the coming decade (e.g. PARASOL, EarthCARE). The utility of such observations for pollution monitoring, air quality forecasting and other operational applications will be evaluated through assimilation by ECMWF, national met services and research institutes during the coming decade.
An identifiable advance for aerosol sounding would be to combine "multi-angle viewing" in the orbitplane (i.e. along the sub-satellite track) with "polarisation sensitivity", as will be done by the Aerosol Polarimeter Sensor (APS) on NPOESS. This is designed to add refractive index, single-scatter albedo and (non-)sphericity information to that on aerosol optical thickness and effective radius which would be supplied by VIIRS alone.
If a similar aerosol polarimeter sensor was deployed in parallel on a Sentinel platform, that could double the geographical sampling of cloud-free scenes per day by APS on NPOESS. If a sun-synchronous orbit with distinctly different (late afternoon) equator crossing time was selected, that could further increase value for air quality forecasting.
A multi-angle polarising sensor deployed in a dedicated Sentinel mission could therefore contribute tropospheric aerosol information of relevance to all application areas, in spite of being non-compliant on horizontal sampling, to supplement that from MetOp/NPOESS.
Eumetsat might wish to consider an aerosol sensor of this type for the post-EPS system.

6.4.4 Nadir UV/VIS/NIR/SWIR

Downward-viewing grating spectrometers to measure backscattered sunlight at uv/vis wavelengths will be integral to trace gas detection in the troposphere by the operational observing system. ECMWF, the national met services and other institutes are therefore preparing for operational usage of data from sensors of this type on MetOp/NPOESS by gaining experience from research satellites (i.e. GOME-1 on ERS-2, SCIAMACHY on Envisat and OMI on Aura). This will be consolidated through use of data from GOME-2 on MetOp and OMPS on NPP and NPOESS.

For air quality and ozone/uv applications, the MetOp/NPOESS system would be augmented in two ways by deploying such a spectrometer on a dedicated Sentinel mission:

(a) Equator daytime crossing-time in later afternoon: therefore closer than MetOp/NPOESS (9:30am / 1:30pm) to early morning AQ and UV forecast times while still sunlit at northern mid-latitude in winter
(b) Smaller ground-pixel size: to sample more frequently between clouds than GOME-2/OMPS. For climate applications, the operational system would be augmented by:
(c) Optional addition of two SWIR channels: for (a) CH_4 and CO detection in the lower troposphere near 2.3 µm and (b) aerosol height-information exploiting relatively strong absorption features of H_2O/CO_2 near 2.0 µm

2-D array detector technology is relatively mature in the uv/vis so, in this wavelength range, only a modest development of the OMI concept is envisaged. The option to add near-IR channels at 2.0 and 2.3 microns would build on experience from SCIAMACHY and would exploit recent advances in HgCdTe array technology, but would require some development and would drive instrument requirements.

6.4.5 Nadir-FTIR

Downward-viewing Fourier transform spectrometers to measure thermal emission at mid-IR wavelengths will be integral to temperature and humidity sounding in the absence of clouds and therefore to the operational observing system for NWP. By measuring the strongest (fundamental)

vibrationrotation bands of trace gases such as CH_4, CO and O_3 they will also provide tropospheric information for the climate and air quality applications under study in CAPACITY.
Geographical and temporal sampling of the cloud-free lower troposphere by IASI and CrIS in the MetOp/NPOESS operational system will be denser than for GOME-2/OMPS in the uv/vis, for two reasons:

1. Night-time as well as day-time sampling
2. Circular fields-of-view of comparatively small diameter (12km for IASI, 14km for CrIS).

Furthermore, the photochemical lifetimes of these trace gases in the troposphere are rather longer than those of NO_2 , SO_2 and H_2CO, which are observed in the uv/vis. The increase in spatio-temporal sampling of CH_4 , CO and O_3 attainable from an additional FTIR on a dedicated Sentinel platform would therefore be somewhat less significant than for an additional uv/vis spectrometer. For O_3 in particular, theoretical simulations indicate that addition of co-located IR spectral measurements could potentially "sharpen up" the tropospheric averaging kernels from uv backscatter measurements alone. The combination of IASI with GOME-2 on MetOp will allow this concept to be investigated in practice. With respect to climate and air quality applications, further value could also be added to the operational system by an FTIR spectrometer if spectral-resolution could be increased (for more accurate trace-gas measurements and detection of additional non-methane hydrocarbons) without compromising across-track sampling.
It can confidently be assumed that Eumetsat will deploy an advanced nadir-viewing FTIR spectrometer in the post-EPS system for NWP. Assuming that the value of IASI to climate and air quality applications is also demonstrated to be high, Eumetsat might wish to consider an FTIR design post-EPS which better addresses these application areas.

6.4.6 Limb-UV/VIS/NIR/SWIR

The OMPS instrument to fly on the two NPOESS platforms in 13:30 daytime equator crossing will incorporate a spectrometer to measure sunlight scattered from the atmospheric limb in a set of tangentheights spaced at 1km in a wavelength range from 290-1000 nm with spectral resolution varying from 1.5 to 40 nm (see Chapter 3 on current and planned missions), designed to be sufficient for stratospheric ozone retrieval using a three-wavelength (Flittner-type) approach. Although height-resolved information on stratospheric aerosol may also be retrieved from tangent-height and wavelength dependence of limb-scattered radiation at "window" wavelengths, spectral resolution may not be sufficient in BrO or NO_2 absorption bands to retrieve stratospheric profiles by applying the DOAS approach to their detailed spectral signatures, as employed by SCIAMACHY and OSIRIS. Furthermore, a recent ESA study (ACOR-2 Final Report, 2005) has shown that to detect aerosol and cirrus in the upper troposphere longer wavelengths are required; optimally 1.041, 1.255. 1.577, 2.065 and 2.251 microns.
A limb-imaging uv/vis/nir spectrometer with higher spectral resolution than OMPS in BrO and NO_2 absorption bands could therefore potentially offer stratospheric BrO and NO_2 profiles of higher quality than OMPS, which could better serve the needs of users in the "scientific assessment" category for the "ozone/uv" and "climate" applications. Additional channels at wavelengths longer than 1 μm would potentially offer supplementary information on scattering by aerosol and cirrus extending to below the tropopause.
Operational assimilation of limb-uv/vis/nir data by the met services has yet to be demonstrated.

6.4.7 Limb-IR & MM/sub-MM

ECMWF has undertaken "passive" assimilation trials with Envisat MIPAS L2 operational products on temperature, ozone and water vapour which were sufficiently promising to move to "active" assimilation of ozone data within ECMWF's operational forecasting system. ECMWF's variational data assimilation system has also been extended to enable direct assimilation of L1 radiances from MIPAS. Theoretical studies indicate that the assimilation of limb radiances from MIPAS can reduce analysis errors for stratospheric temperature, ozone and water vapour, and first assimilation trials with MIPAS radiances support this finding. Steps have also been taken by ECMWF in collaboration with

the Department of Meteorology, University of Edinburgh, towards similar radiance assimilation for Aura MLS, for which it is anticipated that useful information should extend to below the tropopause. Building on experience from the assimilation of Envisat MIPAS and Aura MLS data, temperature, ozone and water vapour data from a future limb-sounding mission would be incorporated into the ECMWF assimilation system used for operational forecasting and those of other met services.
Satellite observations from the limb perspective could also add further value to the MetOp/NPOESS operational system for pollution monitoring and air quality forecasting applications, as follows:
The operational observing system on its own can offer no height-resolution on most trace gases, and only coarse (>5km) height-resolution in the upper troposphere and stratosphere on ozone. To monitor pollution and to forecast air quality it would be highly desirable to discriminate trace gas and aerosol concentrations in the boundary layer and lower troposphere from those in the middle and upper troposphere and stratosphere. Attribution of the height-integrated measurements by nadir-sounders into different atmospheric layers will be controlled entirely by the model representation into which the data is assimilated. Access to high-quality height-resolved information from limb-emission sounding would allow trace gas and aerosol distributions will be represented more accurately through the stratosphere and upper troposphere and (in the absence of cloud) down into the mid-troposphere, allowing information from nadir-sounders to be attributed specifically to the lower troposphere/ boundary layer.
Mm-wave and IR limb-emission techniques offer complementary attributes:

Tropospheric penetration: For trace gases measured in common (e.g. H_2O and O_3), mm-wave is insensitive to cirrus and therefore has a high probability of observing the upper troposphere, whereas IR offers visibility in cloud-free scenes down into the mid-troposphere.

Aerosol and PSCs: Observations at mm-wavelength are completely insensitive to these constituents, which is highly desirable for trace gas retrievals, however, information on aerosol and PSCs is also needed and can be retrieved from observations at IR wavelengths.

Temperature: Observations at mm-wavelengths are much less sensitive to errors in knowledge of atmospheric temperature, which is highly desirable for trace gas retrievals. However, accurate information on temperature is needed too and can be retrieved from observations at IR wavelengths.

Additional trace gases: Observations at mm-wavelengths also target CO and ClO, which are key species in the UT and LS, respectively, whereas those at IR wavelengths also target CH_4 and non-methane hydrocarbons in the UT and LS, together with other species of importance in the stratosphere, e.g. CFCs, HCFCs, NO_2 and $ClONO_2$. Both techniques also target HNO_3.

The mm-wave and IR limb-sounder concepts MASTER and AMIPAS have been studied extensively by ESA in the context of an Explorer class mission. Either concept could directly meet a number of user requirements for ozone/uv and climate applications and, in combination with MetOp/NPOESS via limb-nadir synergy, also enable those for pollution monitoring and air quality forecasting applications to be met better than by MetOp/NPOESS alone.

Definition of instrument requirements for the UTLS limb-sounding component of an atmospheric monitoring, i.e. Sentinel class, mission will benefit further from experience gained by:

- ECMWF and other centres from operational assimilation of temperature, ozone and water vapour data from Aura MLS and from Envisat MIPAS in a new operating mode.
- More extensive demonstration of the limb-nadir synergy concept, through combined use of MIPAS and GOME-1/SCIA O_3 data and application to other trace gases.

6.5 Criteria and Approach for Implementation

It is evident that a dedicated instrument of each of the types discussed in 6.4 could add to MetOp/NPOESS capabilities to address requirements for one or more user category and application area. However, the philosophy of GMES, and therefore the objective of the CAPACITY study, is to define a programme which will serve the future needs of users in the most economical and cost-effective manner. This can best be achieved through exploitation of, and integration with, the MetOp/NPOESS and ground observing systems as efficiently as possible. The following criteria have been considered in devising a step-wise, incremental approach towards a future atmospheric monitoring system which could better serve the needs of users in all categories for all application areas:

1. Whether an MetOp/NPOESS capability will exist at all and, if so, the degree of non-compliance with observational requirements specified for CAPACITY (Chapter 3 Assessment of existing and planned missions)
2. The extent to which major non-compliances by MetOp/NPOESS could realistically be mitigated
3. According to ESA guidance, the needs of users for operational 'NRT services' and 'Protocol Monitoring' aspects are to be assigned higher priority in CAPACITY, and therefore more urgent, than those for 'Assessments'
4. For early implementation as a Sentinel mission, the technical concept must be mature and already demonstrated in space, i.e., only modest further technical development (i.e. risk, time and cost) can be accommodated

6.5.1 MetOp/NPOESS capabilities and degree of (non)-compliance

Table 3.1 in Chapter 3 (Section 3.4) outlines MetOp/NPOESS non-compliances with respect to the data requirements set in Chapter 2. This summary table is based on the analysis of instrument capabilities carried out as part of that task and as detailed in Chapter 3.

6.5.2 Mitigation of major non-compliances

The baseline operational observing system constituted by MetOp/NPOESS could, in principle, be augmented in three physical dimensions:

1. Geometrical

- MetOp/NPOESS is devoid of limb-viewing emission sounders
  - Deployment of limb-emission sounders could provide height-resolved observations in UTLS which would: (a) remedy a major non-compliances for the climate application; (b) provide data of higher quality for ozone/uv application; (c) through limb-nadir synergy, mitigate non-compliances on tropospheric data
- MetOp/NPOESS is devoid of solar occultation sensors
  - Deployment of IR and UV/VIS solar occultation sensors would be highly beneficial to the scientific assessment user category for the ozone/uv application
- MetOp/NPOESS sampling of the boundary layer is limited by GOME-2/OMPS ground pixel size
  - Deployment of a nadir-UV-VIS spectrometer with smaller ground pixel size (while retaining similar swath and sensitivity) would automatically increase by 50% sampling of boundary layer for pollution monitoring / air quality forecast application
- NPOESS will deploy a multi-angle polarising aerosol sensor (APS) in only one orbit
  - Aerosol optical thickness and size will be provided by VIS/IR imagers on MetOp/NPOESS. Deployment of an APS in an additional orbit could double the number of observations of additional aerosol physical properties.

2. Spectral

- MetOp/NPOESS spectrometers do not cover the near-IR
  - Addition of near-IR channel(s) to a nadir-uv/vis spectrometer could provide: (a) additional information on tropospheric CH and CO, through synergy with nadir-FTIR (sensitivity is distinctly different for near-IR and mid-IR), and (b) tropospheric aerosol resolved into several tropospheric layers. Both capabilities would better serve needs of users in all three categories for the climate application.
- Spectral resolution limits MetOp/NPOESS nadir-FTIR spectrometers data quality on CO and other trace gases for climate and pollution/air quality applications
  - Deployment of an FTIR with higher spectral resolution than IASI/CrIS (retaining comparable ground-pixel size, swath and sensitivity), would provide data of higher quality on CO and enable other NMHCs to also be targeted.
- Spectral resolution of OMPS-limb limits quality of height-resolved stratospheric data quality on BrO and perhaps also NO_2, and spectral coverage does not permit scattering by aerosol or cirrus to be measured below the tropopause.
  - Deployment of limb-UV/VIS/NIR with (a) higher spectral resolution in BrO and NO bands and (b) coverage extended to 1 - 2 µm (SWIR) range would reduce non-compliances for scientific assessment categories for Stratospheric Ozone/UV and Climate.

3. Temporal

- MetOp/NPOESS nadir-UV/VIS spectrometers make observations at two local times: 9:30am and 1:30pm
  - Observations in late afternoon of trace gas pollutants in the boundary layer and ozone profiles could have a greater impact on the quality of air quality and surface UV forecast the following morning.

Tables 6.3 and 6.4 outline the potential contribution that can be made by various measurement techniques to the applications identified in this study.

6.5.3 Prioritisation of user categories

ESA guidance is to assign lower priority to the application of data for scientific ‘Assessments’ than for ‘Protocol Monitoring’ and ‘NRT services’.

Application	User category		Degree of Metop/NPOESS non-compliance	Notes
Ozone/UV	Protocol	A1S		
	Operational	A2S	Absence of stratospheric data	1
	Assessment	A3S	Absence of stratospheric data	1
Pollution monitoringand AQ forecast	Protocol	B1S	Serious non-compliances on vertical resolution, horizontal & temporal sampling of troposphere	2,3
	Operational	B2S	Absence of data after 1:30pm; serious non-compliances on vertical resolution & horizontal sampling of troposphere	3,4
	Assesment	B3S	Absence of data after 1:30pm; serious non-compliances on vertical resolution & horizontal sampling of troposphere	3,5
Climate	Protocol	C1S	Lack of boundary layer sensitivity for CO, CH_4 & CO_2 and aerosol sensitivity in mid-stratosphere	
	Operational	C2S	Absence of profile data in upper troposphere & stratosphere	5
	Assessment	C3S	Absence of profile data in upper troposphere & stratosphere	5

Degree of MetOp/NPOESS non-compliance:	**major**	**significant**	**none**

Major *= Key measurements will not be made by MetOp/NPOESS in required height-range and/or time of day*
Significant *= Key measurements made by MetOp/NPOESS will seriously non-comply in vertical resolution, horizontal and/or temporal sampling or precision.*

Notes:

1. *The only stratospheric data to be supplied by MetOp/NPOESS will be that from OMPS-limb on O_3 and possibly aerosol and NO_2. (Assimilation of data from this type of instrument has not yet been demonstrated by ECMWF or other operational centres.)*
2. *Absence of data later than the 1:30pm OMPS measurement will compromise detection and attribution of pollution episodes occurring in the afternoon and so impact on monitoring of adherence to conventions on long-range transport of air pollution.*
3. *Resolution of height-integrated measurements into atmospheric layers (PBL/free troposphere/stratosphere) wholly dependent on assimilation model vertical structure functions for virtually all constituents.*
4. *Absence of data later than the 1:30pm OMPS measurement will compromise the detection of pollution episodes occurring in the afternoon so impact on the early morning AQ forecast*
5. *Data from ADM-Aeolus or EarthCARE lidar could mitigate MetOp/NPOESS non-compliance on aerosol profile in the troposphere, but assimilation yet to be demonstrated.*

Table 6.3. MetOp/NPOESS non-compliance summary table based on WP2200.

Theme	User Category	Code	ir & uv/vis occultation	Limb-mm	Limb-FTIR	Limb UVV-NIR	Nadir-FTIR	Nadir UVV-SWIR	Multi-angle polarimeter	Lidar
Ozone/UV	Protocols	A1S								
	NRT	A2S								
	Assessments	A3S								
Pollution monitoring and AQ forecast	Protocols	B1S								
	NRT	B2S								
	Assessments	B3S								
Climate	Protocols	C1S								
	NRT	C2S								
	Assessments	C3S								
Notes			1	2	2	3	4	5	6	7,8

Value added by new instruments in polar orbit to the operational observing system MetOp/NPOESS

Contribution:	major	significant	some

Major = Unique contribution, ie no measurement of this type otherwise planned in MetOp/NPOESS time frame
Significant = Value added to height-resolution, tropospheric sensitivity and/or timeliness (where crucial for NRT)
Some = Value added only through increasing the *number* of samples per day

- For NRT user categories (A2S, B2S, C2S), square brackets **[..]** means that assimilation by an operational centre not yet demonstrated
- The eight brief accompanying notes indicate how a judgement has been reached on potential added value. The basis for each is discussed in more detail in the report.

Notes:

1. *On the basis of previous missions, it can be expected that ir & uv/vis solar occultation would continue to offer major contributions to long-term monitoring of stratospheric constituent profiles for the assessment categories of ozone/uv (A3S) and climate (C3S) applications, in spite of their geographical sampling limitations.*
2. *There are currently no planned limb-emission sensors beyond Odin, Envisat & Aura. Limb-emission measurements by either mm/submm or FTIR would therefore provide a unique view of the UT & LS complementary to that of the MetOp/NPOESS operational system. This is judged to be a major contribution to NRT and assessment categories for the climate (C2S, C3S) and ozone/uv (A2S, A3S) applications and a significant contribution to the pollution monitoring / air quality application (B1S, B2S & B3S) and the climate protocol monitoring (C1S) application, through direct observations and via limb-nadir synergy.*
3. *A limb-uv/vis/nir instrument additional to OMPS on NPOESS could offer a significant contribution in the assessment category of the ozone/uv application (A3S) by providing height-resolved stratospheric BrO profiles, for which the spectral resolution of OMPS may not be sufficient. It could also provide stratospheric* NO_2 *and aerosol profiles of direct and indirect use (via limb-nadir synergy) to a number of other applications (A2S, B1S, B2S, B3S, C1S, C2S, C3S) by adding to OMPS sampling.*
4. *The value of nadir-FTIR has been gauged specifically as an addition to IASI and CrIS, which will fly on MetOp and NPOESS, respectively, in (at least) two different orbits. There would be some added value from sampling the troposphere more frequently. If a higher spectral resolution than IASI or CrIS could be achieved with a comparable ground pixel size and swath-width and user requirements for the pollution monitoring / air quality forecasting application had been placed on trace gases (eg non-methane hydrocarbons) which are not expected to be detectable at IASI/CrIS spectral resolution, the additional value would become significant. This would also be the case if MetOp was to demonstrate that GOME-2* O_3 *profile retrieval in the troposphere could be improved through synergistic combination with co-located IASI measurements.*
5. *A nadir-uv/vis spectrometer flying in late afternoon orbit (3:30pm) would observe much closer in time than GOME-2 (9:30am) or OMPS (1:30pm) to the early morning forecast times for both air quality (B2S) and surface uv (A2S) and would detect pollution episodes occurring later in the day for protocol monitoring (B1S) and assessment (B3S). These are considered to be major contributions. By adopting a ground-pixel size smaller than GOME-2 or OMPS, cloud-free sampling of the boundary layer would be increased by substantially more than 50% per day. For the climate application, inclusion of near-IR channels sensitive to* CH_4 *and CO in the lower troposphere and to aerosol in several tropospheric layers would offer a major contribution in the protocol monitoring (C1S) category and significant contributions in the NRT (C2S) and assessment (C3S) categories.*
6. *While vis/ir imagers on MetOp/NPOESS should provide adequate data on aerosol optical thickness and size, measurements with greater accuracy over land and of other aerosol properties (eg differentiation of fine/coarse mode, single-scatter albedo) by an aerosol polarising, multi-view sensor flying in a different orbit to APS on NPOESS could add some value for air quality and climate applications*
7. *The ADM-Aeolus or EarthCARE lidar should provide tropospheric aerosol profile data in the MetOp/NPOESS timeframe. Another lidar flying in a different orbit could add some value for air quality and climate applications.*
8. *DIAL is not considered because this technology is undemonstrated in space and not sufficiently mature.*

Table 6.4. Contributions of Measurement Techniques to applications as a function of theme and user category

User Category	Theme	Code	ir & uv/vis occultation	Limb-mm	Limb-FTIR	Limb UVV-NIR	Nadir-FTIR	Nadir UVV-SWIR	Multi-angle polarimeter	Lidar
Protocols	Ozone/UV	A1S								
	Pollution /AQ	B1S								
	Climate	C1S								
NRT	Ozone/UV	A2S								
	Pollution /AQ	B2S								
	Climate	C2S								
Assessments	Ozone/UV	A3S								
	Pollution /AQ	B3S								
	Climate	C3S								
Notes			1	2	2	3	4	5	6	7,8

Value added by new instruments in polar orbit to the operational observing system MetOp/NPOESS

Contribution: **major** **significant** **some**

Major = Unique contribution, ie no measurement of this type otherwise planned in MetOp/NPOESS time frame
Significant = Value added to tropospheric sensitivity, height-resolution and/or timeliness (where crucial for NRT)
Some = Value added only through increasing number of samples per day

- For NRT user categories (A2S, B2S, C2S), square brackets **[..]** => assimilation by operational centre not yet demonstrated
- The eight brief accompanying notes indicate how a judgement has been reached on potential added value. The basis for each is discussed in more detail in the report.

Notes:

1. *On the basis of previous missions, it can be expected that ir & uv/vis solar occultation would continue to offer major contributions to long-term monitoring of stratospheric constituent profiles for the assessment categories of ozone/uv (A3S) and climate (C3S) applications, in spite of their geographical sampling limitations.*
2. *There are currently no planned limb-emission sensors beyond Odin, Envisat & Aura. Limb-emission measurements by either mm/submm or FTIR would therefore provide a unique view of the UT & LS complementary to that of the MetOp/NPOESS operational system. This is judged to be a major contribution to NRT and assessment categories for the climate (C2S, C3S) and ozone/uv (A2S, A3S) applications and a significant contribution to the pollution monitoring / air quality application (B1S, B2S & B3S) and the climate protocol monitoring (C1S) application, through direct observations and via limb-nadir synergy.*
3. *A limb-uv/vis/nir instrument additional to OMPS on NPOESS could offer a significant contribution in the assessment category of the ozone/uv application (A3S) by providing height-resolved stratospheric BrO profiles, for which the spectral resolution of OMPS may not be sufficient. It could also provide stratospheric* NO_2 *and aerosol profiles of direct and indirect use (via limb-nadir synergy) to a number of other applications (A2S, B1S, B2S, B3S, C1S, C2S, C3S) by adding to OMPS sampling.*
4. *The value of nadir-FTIR has been gauged specifically as an addition to IASI and CrIS, which will fly on MetOp and NPOESS, respectively, in (at least) two different orbits. There would be some added value from sampling the troposphere more frequently. If a higher spectral resolution than IASI or CrIS could be achieved with a comparable ground pixel size and swath-width and user requirements for the pollution monitoring / air quality forecasting application had been placed on trace gases (eg non-methane hydrocarbons) which are not expected to be detectable at IASI/CrIS spectral resolution, the additional value would become significant. This would also be the case if MetOp was to demonstrate that GOME-2* O_3 *profile retrieval in the troposphere could be improved through synergistic combination with co-located IASI measurements.*
5. *A nadir-uv/vis spectrometer flying in late afternoon orbit (3:30pm) would observe much closer in time than GOME-2 (9:30am) or OMPS (1:30pm) to the early morning forecast times for both air quality (B2S) and surface uv (A2S) and would detect pollution episodes occurring later in the day for protocol monitoring (B1S) and assessment (B3S). These are considered to be major contributions. By adopting a ground-pixel size smaller than GOME-2 or OMPS, cloud-free sampling of the boundary layer would be increased by substantially more than 50% per day. For the climate application, inclusion of near-IR channels sensitive to* CH_4 *and CO in the lower troposphere and to aerosol in several tropospheric layers would offer a major contribution in the protocol monitoring (C1S) category and significant contributions in the NRT (C2S) and assessment (C3S) categories.*
6. *While vis/ir imagers on MetOp/NPOESS should provide adequate data on aerosol optical thickness and size, measurements with greater accuracy over land and of other aerosol properties (eg differentiation of fine/coarse mode, single-scatter albedo) by an aerosol polarising, multi-view sensor flying in a different orbit to APS on NPOESS could add some value for air quality and climate applications*
7. *The ADM-Aeolus or EarthCARE lidar should provide tropospheric aerosol profile data in the MetOp/NPOESS timeframe. Another lidar flying in a different orbit could add some value for air quality and climate applications.*
8. *DIAL is not considered because this technology is undemonstrated in space and not sufficiently mature.*

Table 6.5. Contributions of Measurement Techniques to applications as a function of user category and theme.

6.5.4 Instrument design and development status and European experience

IR & uv/vis solar occultation

- Long and successful heritage in US through SAGE-I,-II,-III and HALOE and in Japan through ILAS-I and -II and POAM-I,-II and –III
- Canada also has established experience in solar occultation through ACE and MAESTRO on SCISAT
- On uv/vis side, some experience is also being acquired in Europe from the GOMOS (stellar occultation) and SCIAMACHY (solar occultation mode) experiments on Envisat.

Lidar and DIAL

- The US demonstrated the first space-borne aerosol lidar through LITE on the space-shuttle.
- Experience has been acquired by France through CALIPSO. Experience is being acquired more widely in Europe through the ADM-Aeolus and EarthCARE lidars.
- No spaceborne DIAL instrument has yet been developed, so this technology is not sufficiently mature for consideration as a Sentinel.

Nadir-uv/vis/nir grating

- The US pioneered uv backscatter spectrometry through BUV in the 1970s, followed by the series of TOMS and SBUV sensors, to which the successor will be OMPS on NPP and NPOESS.
- Europe has established an internationally competitive position in instrumentation of this type through GOME-1, SCIAMACHY, OMI (Netherlands) and GOME-2.
- The OMI concept is now demonstrated for uv/vis. Optional addition of nir/swir channel(s) has been studied in the Netherlands, as supplied for this study. This would drive design and require some further development.

Nadir-FTIR

- Provision of IASI to MetOp has established a competitive international position for France in relation to US (TES, CrIS) and Japan (IMG,GOSAT) for this type of instrument.
- Design of an FTIR spectrometer with higher spectral resolution for sounding tropospheric trace gases has been studied in France (e.g. TROC initiative).

Multi-angle polarising sensor

- Through MISR, the US has demonstrated a "multi-angle" along-track viewing aerosol sensor, and this experience is being further consolidated through APS for NPOESS.
- Through the ATSR series, the UK has a track record in "dual-view" vis/ir imagers for sea surface temperature.
- Through POLDER and PARASOL, France has demonstrated across-track scanning polarising uv/vis imagers.
- The Netherlands has experience of pre-flight characterisation and calibration of polarising uv/vis instruments and has performed early studies of a multi-angle polarising sensor, as supplied for this study.

Limb-uv/vis/nir/swir

- The US has a demonstrated capability for this type of sensor, dating back to SME in the early 1980s, consolidated by LORE and SOLSE-1 and -2 on the space-shuttle and now to be advanced further through OMPS on NPP and NPOESS.
- Through OSIRIS, Canada also has an established reputation for this type of instrument.
- Europe has experience through involvement in OSIRIS and build of SCIAMACHY.

Limb-ir & mm/sub-mm

- Through TES and MLS on Aura, the US has demonstrated capability for limb-FTIR and limbmm/submm sounders.
- Through Envisat MIPAS and Odin Sub-Millimetre Radiometer, competitive capabilities have been demonstrated in Europe for both classes of instrument.

6.5.5 Findings

Findings from applying the above four criteria can be summarized as follows:

1. IR & uv/vis solar occultation

- This type of sensor could offer stratospheric profile data of great value to users in the scientific assessment category for climate and ozone/uv applications (in spite of appearing to grossly non-comply on horizontal sampling). However, there would be no "operational" NRT users for this type of data.
- It would therefore be constructive for a new sensor of this type for long-term monitoring of the stratosphere to be led by US, Canada or Japan, where specialist expertise is much better established than in Europe.

2. Lidar and DIAL

- Although the passive instruments on MetOp/NPOESS cannot supply tropospheric profile information on aerosol, the lidars on ADM-Aeolus and EarthCARE will mitigate this deficiency.
- Development of a dedicated aerosol lidar is therefore not considered the highest priority for an early Sentinel mission but might be a candidate for post-EPS, following evaluation by ECMWF other operational centres of ADM-Aeolus
- DIAL technology is not yet sufficiently mature to be considered for a Sentinel mission.

3. Nadir-uv/vis/nir/swir grating

- Deployment of a nadir-UV-VIS-NIR-SWIR spectrometer in late afternoon orbit offers an attractive prospect for pollution monitoring / air quality forecasting and for Stratospheric Ozone/surface UV applications, for two reasons
  (a) There would be an unambiguous and large increase in the number of samples per day. Depending on how much smaller than OMPS (50km×50km) and GOME-2 (40km×40km or 80km×40km) the ground pixel size is, the number of (cloud-free) boundary layer observations would increase by a factor much larger than 50%
  (b) Observations made in late afternoon would be much closer in time, and would therefore be anticipated to have a greater impact on, early morning forecasts of air quality and surface UV.

  Optional addition of SWIR channels near 2.3 and 2.0 µm would offer added value for the climate applications through:
  (a) near-surface CH_4 and CO
  (b) resolution of aerosol in several tropospheric layers in cloud-free scenes, from scattering in strong H_2O and CO_2 bands.
- European technical expertise in building this type of instrument is internationally competitive and a mature concept exists for UV/VIS, through OMI.
- Technical development would be required for addition of near-IR channels. However, this would benefit directly from new HgCdTe detector arrays and recent experience in Netherlands gained from re-evaluation of SCIAMACHY near-IR channel design, pre-flight characterisation and in-flight calibration.

This concept can therefore be recommended for immediate Phase A study.

3. Nadir-FTIR

- Although it is assumed that IASI and CrIS will be flying in parallel in at least two polar orbits (therefore sampling at least four times of day), deployment of a dedicated nadir-FTIR spectrometer with higher spectral resolution but similar swath / pixel size would be a useful addition to uv/vis/nir grating spectrometer in late afternoon orbit
  - (a) increase (by up to 50%) in density of sampling per day from IASI + CrIS
  - (b) detection of additional trace gases (e.g. NMHCs although requirements for these were not made specific in Chapter 2). So, although a stand-alone nadir-FTIR instrument could add some value to MetOp/NPOESS, this is gauged to be much less significant than a stand alone nadir-UV-VIS-NIR spectrometer.
  - (c) the further added value which might come through synergy with co-located uv for tropospheric O_3 profiling is to be assessed from 2007 onwards using IASI in combination with GOME-2 on MetOp.
- Following successful demonstration of IASI, Europe, and particularly France, would be well-positioned to develop a new instrument of this type as an evolution of IASI post-EPS.

5. Multi-angle polarimeter

- Addition of a second multi-angle aerosol polarimeter flying in parallel to APS on NPOESS could be useful for physical properties additional to aerosol optical thickness and size.
- With lead in sensors of this type firmly with the US, parallel development in Europe would not be the most cost-effective use of Sentinel budget to monitor atmospheric composition.

6. Limb-uv/vis/nir/swir

- A limb-imaging uv/vis/nir spectrometer with higher spectral resolution than OMPS in BrO and NO_2 absorption bands could potentially offer stratospheric BrO and NO profiles of higher quality than OMPS to better serve the needs of users in the "scientific assessment" category for the "ozone/uv" and "climate" applications. Additional channels at wavelengths longer than 1 µm could offer supplementary information on scattering by aerosol and cirrus extending to below the tropopause.
- However, operational centres have not yet demonstrated usage of this type of data and the US (through OMPS) and Canada (through OSIRIS) have demonstrated capabilities, so parallel development in Europe would not be the most cost-effective use of Sentinel budget to monitor atmospheric composition.

7. Limb-ir & mm/sub-mm

- There will be no limb-emission sensor on MetOp/NPOESS and the limb-emission sensors on Odin, Envisat and Aura are unlikely to function beyond 2010.
- Deployment of limb-emission sounders could provide height-resolved observations in UTLS which would: (a) remedy non-compliances for the climate application; (b) better address requirements for the Stratospheric Ozone/Surface UV applications; (c) directly and indirectly, through limb-nadir synergy, mitigate non-compliances on tropospheric data
- An operational centre (ECMWF) has demonstrated a positive impact from Envisat MIPAS assimilation and is currently undertaking similar trials with Aura MLS.
- Europe is competitive with US with respect to both IR and MM/sub-MM limb-emission sounders and there are no US plans for either at present.

In preparation for a future UTLS limb-sounding component, it is therefore recommended to:

(a) evaluate impact assessments of Aura MLS assimilation and further Envisat MIPAS assimilation by ECMWF and other centres
(b) demonstrate the value of limb-nadir synergy for pollution monitoring and air quality forecasting with Envisat and Aura data
(c) re-scope limb-mm and limb-IR instrument requirements through quantitative retrieval simulations on the basis of user requirements for monitoring defined in this study and those to be defined by Eumetsat post-EPS.

6.5.6 Specific Recommendations for Assessment of Space Segment Issues (WP3300)

With the limited resource available in WP3300 to assess space segment issues it is recommended that the following be given priority for attention:

Higher Priority

- Nadir-uv/vis/nir
- Limb-FTIR
- Limb-mm

Lower Priority

- Occultation
- Limb-uv/vis/nir
- Nadir-FTIR
- Multi-angle polarising imager
- Lidar

6.6 Overall Recommendations

In accordance with the philosophy of the GMES Sentinel programme as a whole, the atmospheric composition monitoring component should exploit the planned operational observing system constituted by the ground network plus MetOp/NPOESS as extensively as possible and build on this as efficiently and cost-effectively as possible.

The main recommendations are:

1. For evolution through a phased approach from the MetOp/NPOESS system towards a system post-EPS which better serves user needs for monitoring atmospheric composition.

2. To seek to achieve this through co-operation with: the US via reciprocal agreement on NPOESS data access; with US, Canada or Japan for possible provision of a solar occultation mission, in which their heritages are strong, and with Eumetsat on post-EPS definition.

3. As a first step, to undertake a Phase A study leading to implementation of a single dedicated Sentinel platform carrying nadir-viewing instrumentation in an orbit to complement MetOp/NPOESS in 9:30am and 1:30pm daytime equator crossing times, and thereby better serve the needs of operational users in Europe and worldwide for pollution monitoring and air quality forecasting, together with ozone/uv and climate applications. Instrument requirements are indicated in some detail in the Technical Note on this work package, **TN3200**:
   - The specification of a uv/vis/nir spectrometer to address pollution monitoring and air quality forecasting applications may be based on that provided in **Section 1.2.6 of TN3200**, "Nadir UV-VIS-NIR 2D Imaging Spectrometer" – the potential alternative solution of an across-track scanning 1D spectrometer not being excluded.
   - The specification of swir channels centred near 2.35µm to monitor CO and near-surface methane for the climate application and 1.9µm to resolve aerosol into several layers may be based on **Section 1.2.7 of TN3200**, "Nadir-SWIR Grating Spectrometer". The 1.9µm channel has been shown in simulations to offer more potential for height-discrimination than the O_2-A band at 764nm.
   - Sub-pixel cloud identifications indicated in **Section 1.2.7 of TN3200** are also relevant. Sub-pixel cloud detection could potentially be provided by either (a) an integral sensor (e.g. faster read-out of across-track scanner, as per GOME-2 PMDs), or (b) VIIRS imager on NPOESS platform in late afternoon orbit (analogous to MODIS function for Aura nadir-sounders) rather than a separate, stand-alone imager.

4. In parallel, to prepare for a future limb-sounding component:

(a) evaluate the impact of Envisat and Aura limb-sounder data in assimilation by ECMWF and other operational centres – Limb-sounder data has an indirect impact at altitudes below the observed height range in addition to the direct impact in the observed range. It has been demonstrated in both retrieval and assimilation that limb-nadir synergy is beneficial for ozone and it is expected to improve tropospheric data quality for air quality as well as climate and ozone/surface uv applications (studies in support of an Explorer-class mission).

(b) define limb-mm and -ir instrument requirements through quantitative retrieval simulations on the basis of user requirements from CAPACITY for monitoring applications – Limb-sounder specifications available to the CAPACITY study (AMIPAS and MASTER) were as defined by earlier ESA studies in support of an Explorer-class mission.

5. Definition of future nadir- and limb-sounding components, as might be accomplished in cooperation with EUMETSAT or other partners, would benefit from evaluation of:
   (a) nadir-FTIR : IASI and synergy with GOME-2 on MetOp
   (b) limb-uv/vis/nir :OMPS on NPP
   (c) multi-angle aerosol polarimeter : APS on NPP/NPOESS
   (d) tropospheric aerosol lidar : CALIPSO and ADM-Aeolus

7 Evaluation of Critical Space Segment Issues

7.1 Introduction

In the context of the ESA CAPACITY study on the definition of future operational atmospheric chemistry missions the results of this work package (WP 3300) are documented in this chapter. The objective of this activity is to support the definition of mission requirements by analysis

- of alternative mission scenarios including
- of the geostationary mission scenario based on inputs defined in Chapter 5
- of the low earth orbit mission scenario based on inputs defined in Chapter 6

First assessment in form of comparison with earlier and on-going studies and specific simulations with modified parameters are made to outline

- integrity of requirements
- feasibility of mission concepts
- feasibility of instrument concepts

7.2 Mission Analysis

7.2.1 Introduction

Already the study logic and work packages of the Capacity study are showing the parallel investigations of two missions, a geostationary mission and a low earth orbit mission. Herein these chapter first investigations of additional alternative mission scenarios are given. More exotic scenarios e.g. like a Molniya orbit are also considered but not analysed into more detail, because no advantages are noticeable for the discussed applications.

7.2.2 LEO/MEO Satellite Constellation

For Capacity one of the most driving parameter compared to other LEO/MEO applications is the so called revisit time. Especially for Air Quality applications (B1S – B3S) a high observation frequency with revisit time of 0.5 to 2 hrs is required. Looking to conventional LEO/MEO missions with single satellite like ERS-1/2 and ENVISAT the complete earth is covered after 1 to 3 days, depending of the swath width observed by the instruments.

So based on a single satellite in a sun-synchronous orbit the revisit time at the equator can not be increased above 1 observation per day. But using a constellation of 3 satellites improves the situation drastically.

Additional variations of the orbit altitude and maximum instrument Line of Sight (LOS) angle are feasible. In Figure 7.2.2-3 and Figure 7.2.2-4 such constellations are shown for revisit times of the order of 2 hours and 4 hours. In both cases given in Figure 7.2.2-3 and Figure 7.2.2-4 the outer orbit planes of the sun-synchronous polar orbits are +/-60 deg rotated to the inner orbit plane.

Please note that the real revisit time depends also on the orbit period which again is a function of orbit altitude. Also with the phasing of the different satellites in the different orbits the revisit time is effected. So the 2 hours and 4 hours are to be taken as order of magnitude only

Figure 7.2.2-3 shows the 3 satellite configuration and the needed maximum instrument LOS angle for a 2 hours revisit time. For this geometric constellation the LOS angle is shown in Figure 7.2.2-1 in detail. The resulting angle between horizon and instrument LOS, the so called ground elevation angle, is very acute and close to the Limb geometry, not acceptable for Nadir applications. But with an increase of the orbit altitude the situation can be relaxed. The resulting minimum ground elevation angle is shown in Figure 7.2.2-5 as function of orbit altitude for revisit times of 2 and 4 hours.

As reference for the minimum useful ground elevation angle the observation geometry of OMI is given in Figure 7.2.2-2. OMI is launched on the EOS-Aura platform and operated in 705 km altitude. With a viewing angle of +/- 57 deg a Nadir swath of 2600 km is observed. The resulting minimum angle between horizon and instrument LOS is 21 deg. Taking this value as lowest limit the minimum for the ground elevation angle the resulting orbit altitudes are 3090 km for 2 hours (correctly obit period is 2.55 hours) and 985 km for 4 hours (correctly orbit period is 3.46 hours) revisit times, as shown in Figure 7.2.2-5.

Using the geometrical configuration for an optimization of the orbit for higher latitudes than the equator, e.g. for 30 deg latitude, the orbit altitude can be decreased. Full earth coverage can be obtained over Europe as shown in Figure 7.2.2-9, but at the equator gaps have to be taken into account, as given in Figure 7.2.2-8. So with a constellation of 3 spacecrafts in an altitude around 894 km which is close to the conventional sun-synchronous orbits (ERS1/2, ENVISAT, METOP, …) a revisit time in the order of 4 hours is feasible. The correct orbit period is 3.43 hours. The selected local time for descending nodes are 8:00, 12:00 and 16:00. Optionally also with the same local time but for ascending nodes the same coverage can be obtained.

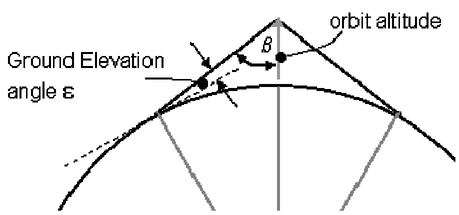

Figure 7.7.2-1. Ground Elevation Angle between horizon and LOS for maximum deflection.

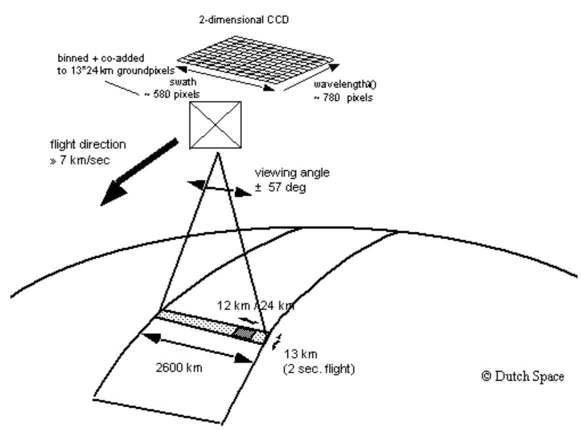

Figure 7.7.2-2. OMI observation geometry, http://www.knmi.nl/omi/research/instrument/index.html

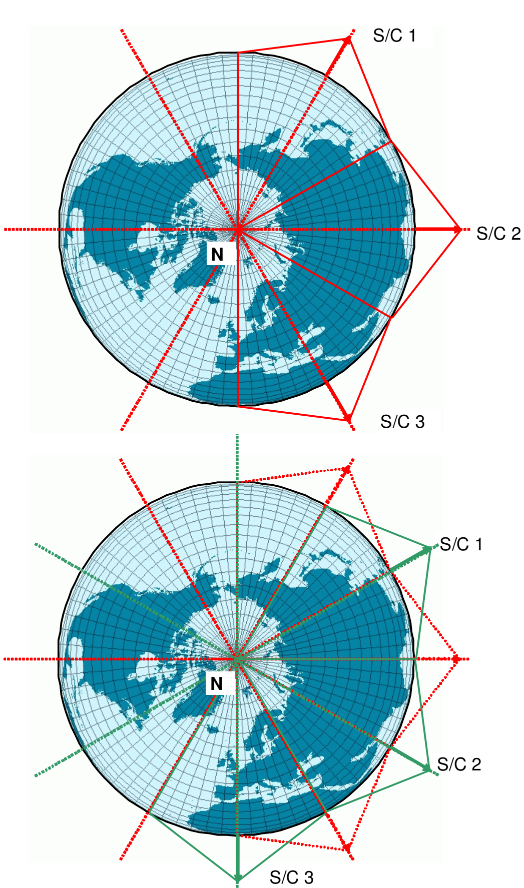

Figure 7.7.2-3. Orbit n (top, red) and orbit n+1 (bottom, green) for 3 spacecraft configurations with full coverage **2 hours** equatorial revisit time of Nadir observations.

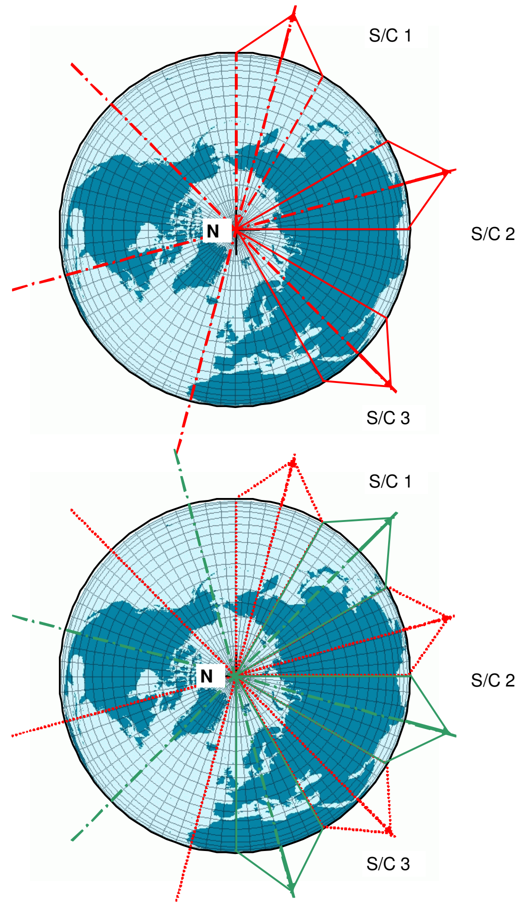

Figure 7.7.2-4. Orbit n (top, red) and orbit n+1 (bottom, green) for 3 spacecraft configurations with full coverage **4 hours** equatorial revisit time of Nadir observations.

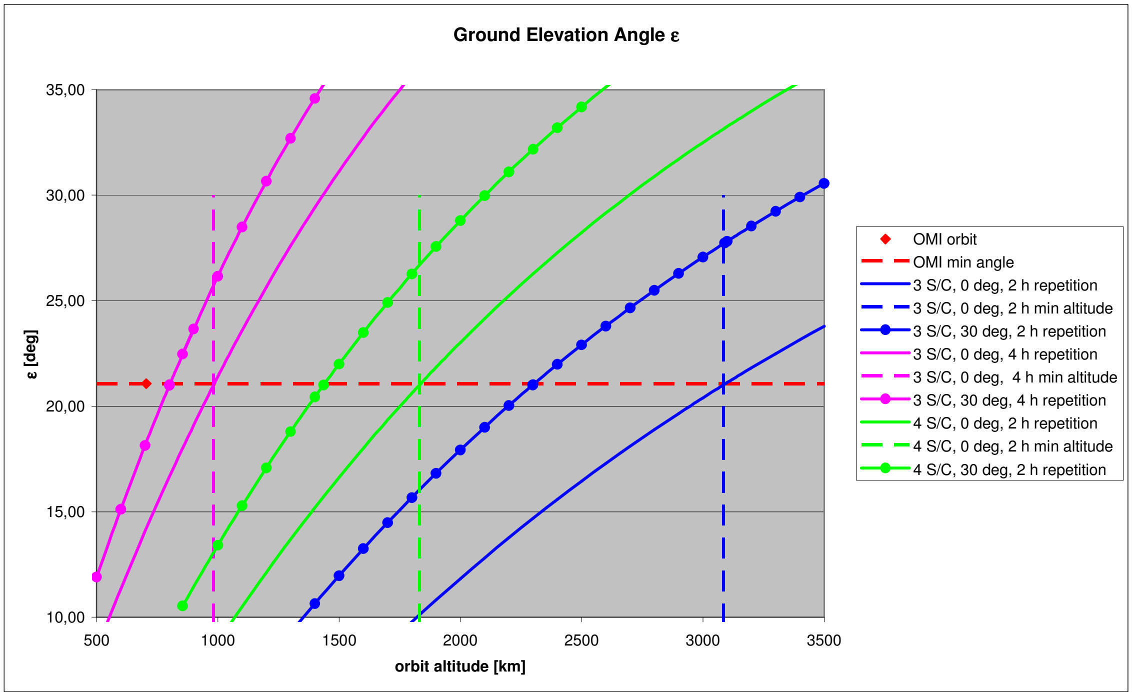

Figure 7.7.2-5. Ground Elevation Angle between horizon and LOS as function of orbit altitude and repetition time for 0 deg and 30 deg latitude (Nadir = 90 deg).

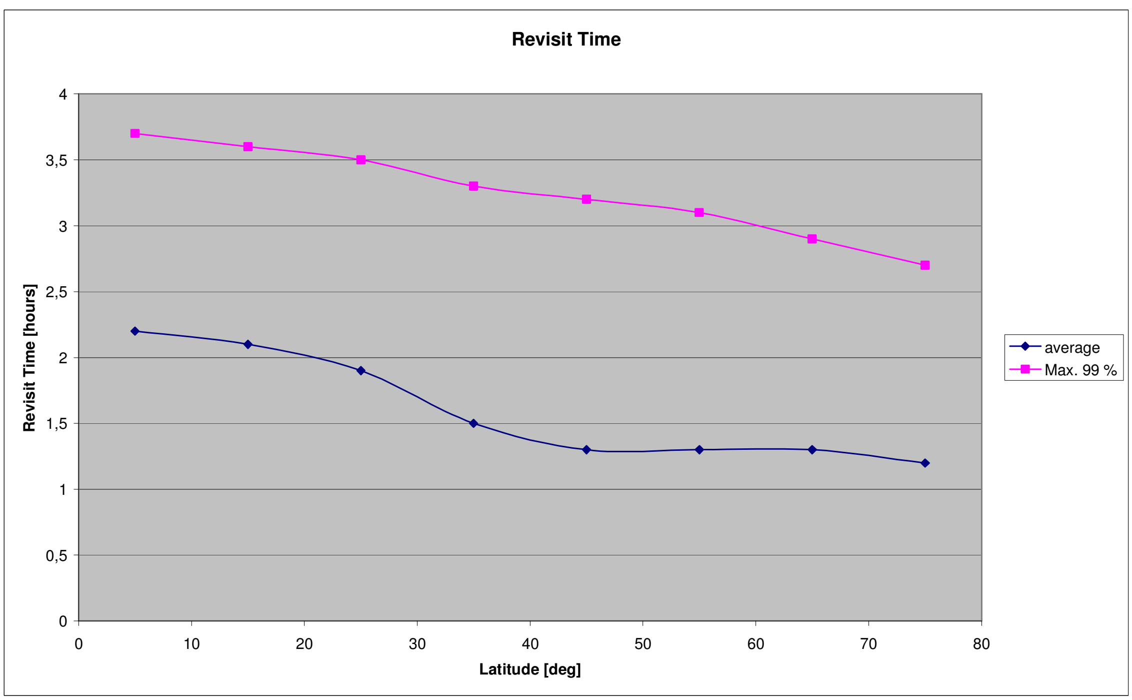

Figure 7.7.2-6. Revisit Time: Average and maximum of 99 % of for 3 spacecrafts, altitude 3000 km.

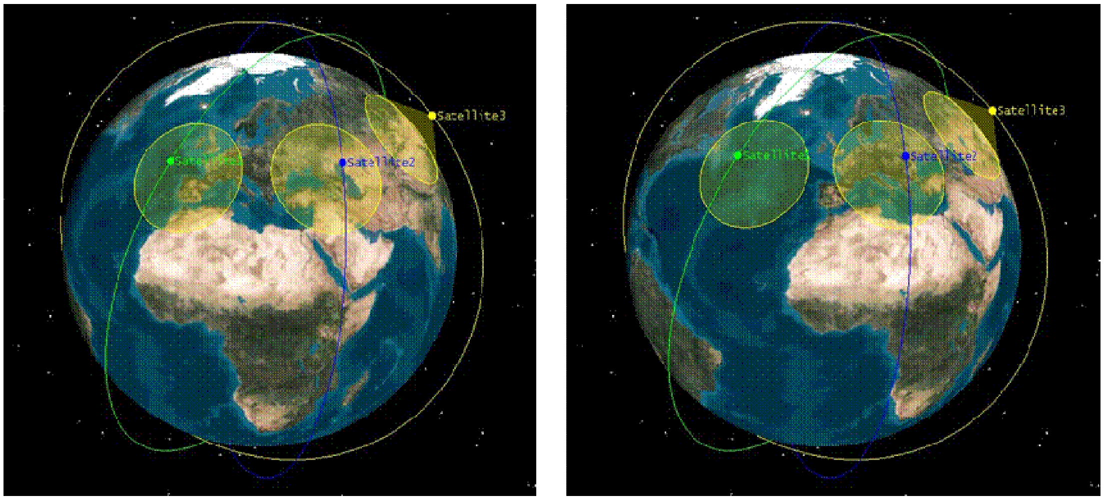

Figure 7.7.2-7. 3 sun-synchronous satellite constellation, orbits 1 and 2

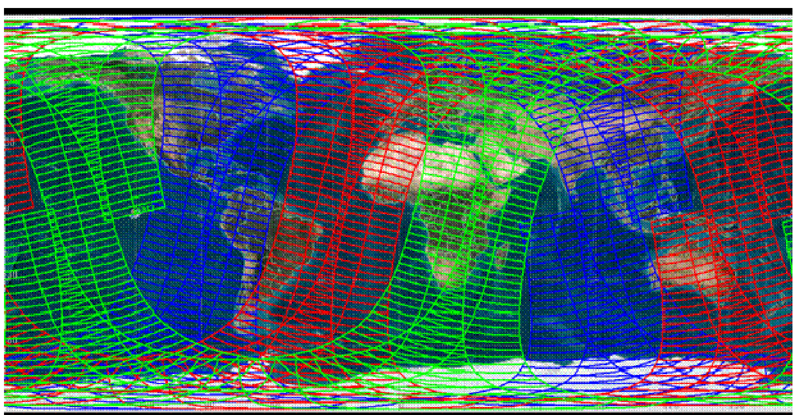

Figure 7.7.2-8. 3 sun-synchronous satellite constellation, orbits 1 and 2, earth coverage.

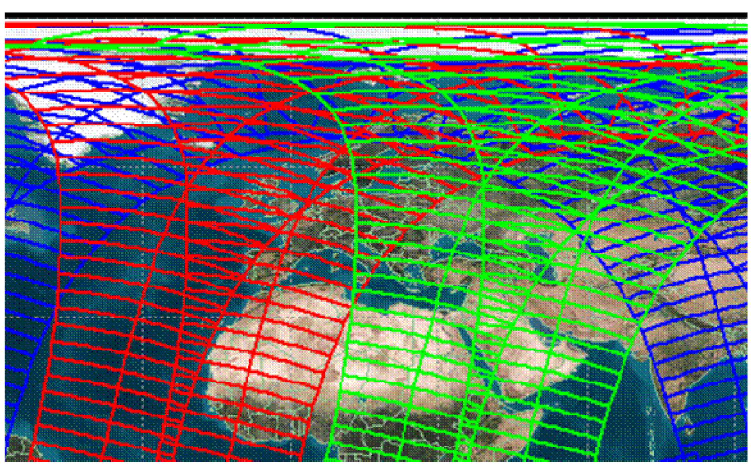

Figure 7.7.2-9. 3 sun-synchronous satellite constellation, orbits 1 and 2, Europe coverage.

7.2.3 Inclined Low Earth Orbit Constellation

As already mentioned above it is an objective to increase the revisit time especially over Europe. So an alternative to the sun-synchronous orbits is to increase the inclination of the circular orbit e.g. to 125 deg. Also for such an orbit a constellation of 3 satellites is needed to obtain continuous earth coverage. But due to the inclination optimized for Europe with such a constellation a repetition time in the order of 2 hours is feasible with moderate orbit altitudes.

For the example given herein also an altitude of 894 km is chosen. In Figure 7.2.3-1 the orbit planes for an inclination of 125 deg are shown.

In Figure 7.2.3-2 and Figure 7.2.3-3 the coverage over Europe is shown in a sequence of 5 and 10 orbits. The same Nadir Elevation angle as defined for OMI has been applied.

The advantages of this class of orbit are:

- Nearly full coverage of Europe is given,
- with an average revisit time of 1.7 hours.
- The local time of the observation varies from orbit to orbit, so diurnal atmospheric variations can be observed.
- A cross-calibration of missions in sun synchronous orbits with different local time is feasible.

But the disadvantages are:

- Due to the strong variation of the geometric observation conditions and local observation time the evaluation of the diurnal effects is more complicated.
- Due to the lower inclination no full global coverage is given.

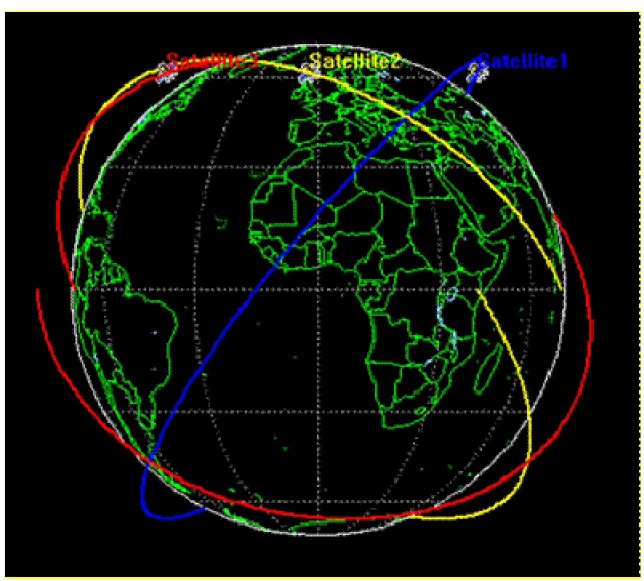

Figure 7.2.3-1. Constellation of 3 satellites with 125 deg inclined orbits, 894 km altitude

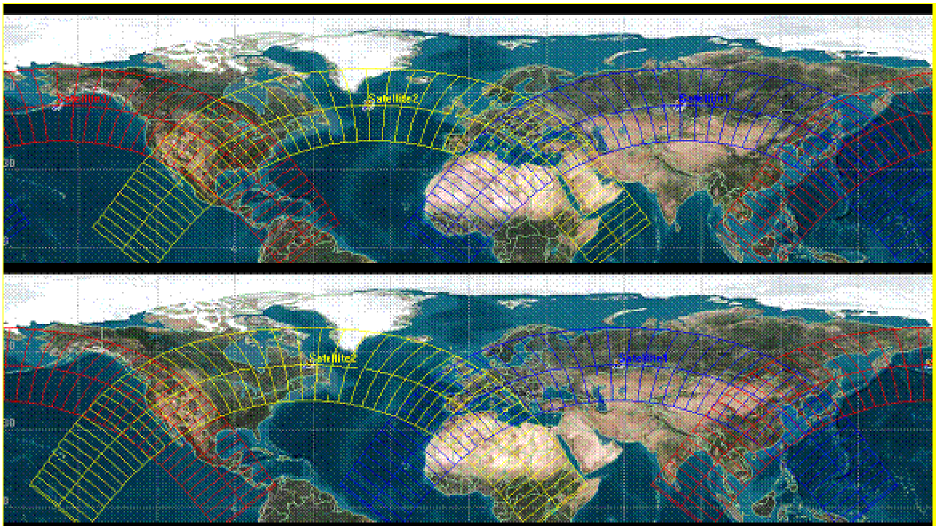

Figure 7.2.3-2. Sequence of inclined orbits (894 km, inclination 125 deg)

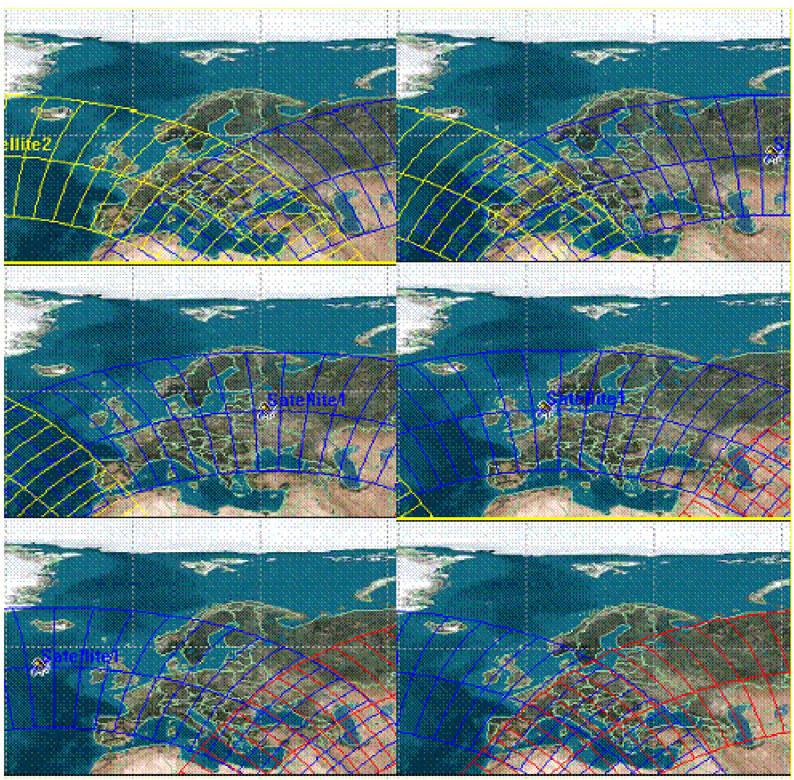

Figure 7.2.3-3. Sequence of inclined orbits: Coverage over Europe for Orbit 1 (894 km, inclination 125 deg)

7.2.4 Radiation environment

For an earth observation mission the most limiting aspect for an orbit selection is the radiation environment. As an example the annual total dose for different circular equatorial orbits is shown in Figure 7.2.4-1. The two maxima are showing the centres of the inner and outer Van Allen Belts.

The particles are distributed such that the inner belt consists mostly of high-energy protons (10-50 MeV) while the outer belt consists mostly of electrons.

As reference the ENVISAT orbit with 800 km altitude is shown. Please note that the absolute values given in Figure 7.2.4.1 are applicable for equatorial orbits only. So for the inclined polar orbits the situation improves. But for a first rough relative assessment the figure is valid.

The resulting orbit altitudes for the 2 hours and 4 hours equatorial revisit time discussed above are also given. Compared to the ENVISAT orbit the total dose increase by a factor of 10 for the 4 hours revisit and a factor of 5000 for the 2 hours revisit constellation.

The figure shows also that the annual total dose for a geostationary orbit is much stronger than for ENVISAT. But as mentioned above the outer belt consists mainly of electrons, the inner belt of protons. Figure 7.2.4-2 shows that a protection by shielding is very effective against damages by electrons but not against protons. Please note that in Figure 7.2.4-1 a 4-mm aluminium shielding is already applied.

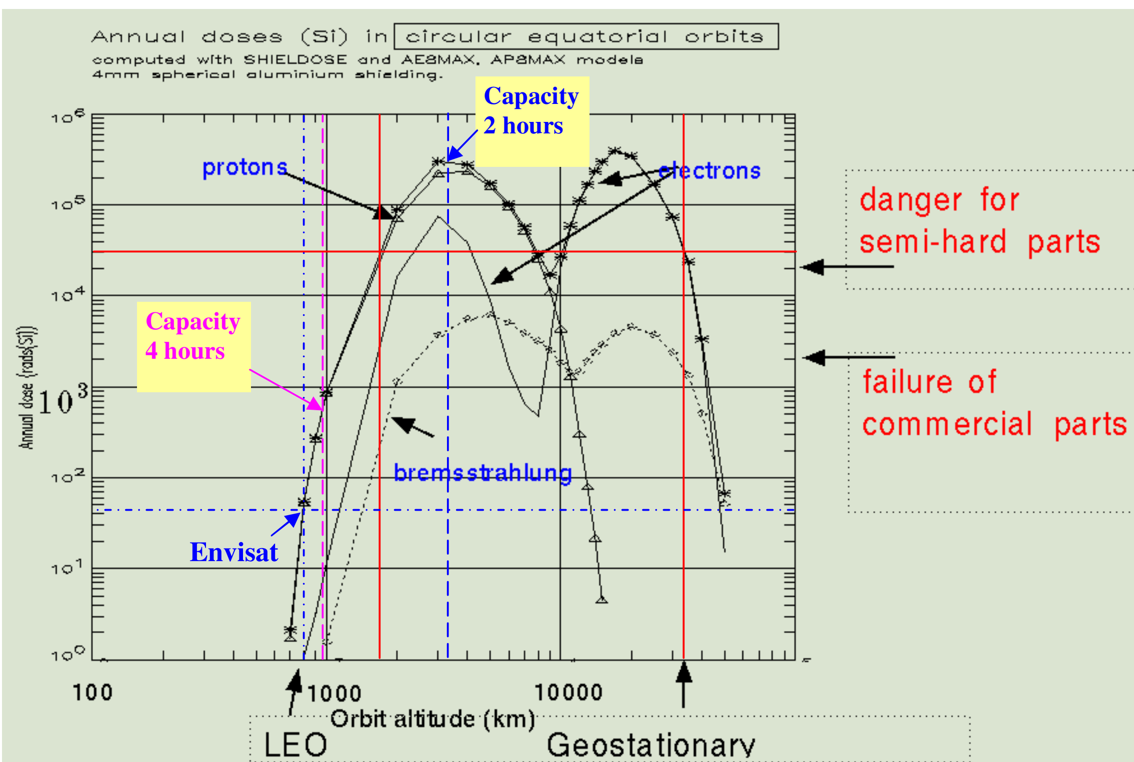

Figure 7.2.4-1. Total dose (annual) for circular equatorial orbits.

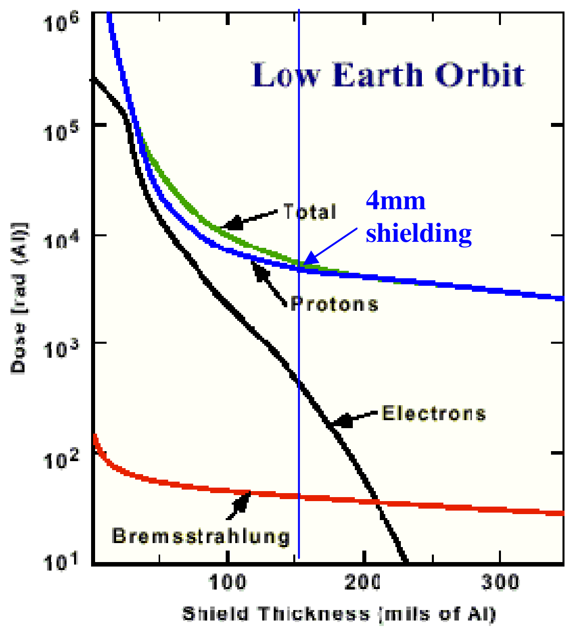

Figure 7.2.4-2. Radiation Shielding(100 mils = 2,54 mm).

7.2.5 Conclusions

Herein this discussion the two most driving and contrary mission requirements are the

- Revisit time, especially locally required over Europe
- The low frequent full earth coverage

In **Error! Reference source not found.** the discussed options with the resulting revisit times and earth coverage are shown.

	No. of satellites	Revisit Time over Europe	Coverage
GEO plus	1 +	continuous	local over Europe
LEO sun-synchronous	1	1 - 3 days	global
LEO sun-synchronous constellation	3 at 894 km	ca 3.4 hours	global
LEO inclined orbit constellation	3 at 894 km	ca 1.7 hours	global up to 75 deg of latitude

Table 7.2.5-1. Discussed mission options

The **Error! Reference source not found.** shows that a dedicated GEO satellite enables an continuous observation over Europe and a dedicated LEO satellite obtains full global coverage with a much longer revisit time. So a combination of both satellites fulfils the main mission requirements best. But it is also obvious that the effort to develop two independent satellites with dedicated instruments is significant. So alternative mission scenarios based on constellations with 3 identical satellites are also presented.

The first analysis described above shows that the revisit time for low earth orbits can be strongly reduced by using a constellation of 3 satellites and/or higher orbit altitude. But the resulting earth coverage is limited by the useful viewing angles for Nadir observations and the earth radiation environment damages increasing with altitude. So a sun-synchronous orbit of 3090 km altitude allows a 2.55 hours revisit time, but for this altitude the total radiation dose can not be handled. So the orbit altitude has to be strongly decreased resulting in longer revisit times. For a constellation of 3 sun-synchronous satellites an orbit altitude of 894 km is recommended. The achieved revisit time over Europe is approximately 3.4 hours.

Such a constellation is only recommended for a combined mission as compromise between the dedicated requirements for the different applications. If e.g. a mission is limited to local protocol monitoring application requiring a high revisit time over Europe the discussed sun-synchronous LEO constellations are no alternatives.

But with respect to the revisit time an alternative mission design is a constellation of 3 satellites in a low inclination orbits. Using the identical altitude and observation geometry (as applied for OMI) the revisit time e.g. of Europe can be strongly decreased to 1.7 hours. This option sounds very attractive and it is recommended to analyse this mission design in more detail with respect to the impacts on the observation performance and spacecraft and instrument design. It has to be noted that e.g. the spacecraft power management becomes more complicate than for a sun-synchronous orbit.

The discussion above shows that the

- geostationary orbit is the optimum for applications requiring <u>short revisit times</u> or quasi-continuous observation with <u>limited earth coverage</u>, e.g. of Europe
- low earth orbit is the optimum if observations of <u>daily</u> and <u>global</u> coverage are required

So the orbit alternatives discussed above are compromises with impact on observation performance which has to be analysed in more detail for the different applications in future studies. So presently a constellation of 3 LEO spacecrafts is only recommended for a combined mission as compromise between the dedicated requirements for the different GEO and LEO applications. Also using the low inclined orbit is to reduce costs with the disadvantage of decreased performance.

If a mission is limited to the protocol monitoring application requiring a higher revisit time over Europe the discussed LEO constellations and the low inclination orbit are no alternatives. On the other side for most of the remaining applications a global coverage with daily revisits is sufficient.

If these contrary requirements shall be covered by a single mission a design optimization has to be performed, taking additional aspects like the measurement principle into account. Due to the fact that during eclipse no backscattering of solar light exists the mission designs optimized dedicated for absorption backscattered or thermal infrared emission measurements are leading to different solutions.

But not only dedicated measurement aspects are driving the selection of a specific mission concept. The objective of Capacity is to identify the needs for future operational atmospheric chemistry monitoring missions. The most important operational mission in Europe is the Meteosat-program.

Presently ESA and EUMETSAT are iterating the mission requirements for the third generation of Meteosat (MTG). Due to the operational character of this mission additional requirements are very important, especially:

- the overall duration of the mission
- the availability of the data
- and the in-orbit spare philosophy for optimized mission reliability.

An example may show the additional impact of these requirements.

In case of a total loss of a single satellite the combined GEO/LEO mission would result in the total loss of data, either on the frequent revisit of Europe or the global coverage. In case of the inclined LEO constellation the orbit plain of the remaining two satellites may be adapted so that a revisit time of better than 3 hours can be maintained.

Also if, e.g. like for MTG, in-orbit spares will be required for the mission design it means that for both satellites of the GEO/LEO mission an additional spare satellite is needed. But in this case the cost impact on the GEO/LEO mission is much stronger than on the LEO constellation for which a single spare satellite is only needed.

Please note that in the following chapters the payload aspects are discussed dedicated for the GEO and for the LEO applications, assuming that no consolidation of both in a single mission will be performed.

7.3 GEO Applications

7.3.1 Mission and Systems Concepts

The need of a geostationary atmospheric chemistry mission is strongly driven by the air quality applications for protocol monitoring, near-real-time and assessments. A revisit time between 0.5 and 2 hours combined with a spatial resolution better than 20 km x 20 km is driving the mission. But the required observations are limited to Europe. So these main requirements can be best fulfilled by a geostationary satellite and is presently not addressed by any existing mission. Initially plans to add an atmospheric mission in form of an UVS instrument on Meteosat Third Generation (MTG) are discarded for programmatic reason.

The air quality applications are the main objectives for the GEO-Mission and are including observations like primary pollutants (e.g. CO, SO_2, NO_2 and volatile organic compounds (VOCs), Oxidants and Aerosol.

Based on the actual requirements and analysis a mission concept similar to the GeoTROPE proposal (Proposals for the Earth Explorer Opportunity Missions, ESA's 2nd Call, 2002) can be expected. Therefore herein this report an overview about the GeoTROPE concept is shortly described as technical reference.

In order to measure the required parameters also GeoTROPE comprises two nadir-looking instruments, a UV-VIS-NIR-SWIR spectrometer (GeoSCIA) and an IR-FTS spectrometer (GeoFIS), mounted on a geostationary platform. The chosen geographic area will cover the European continent, Africa, middle East and surrounding oceans. The area will be covered every 30 – 60 min. with a horizontal sampling of 11.5 x 23 km^2 to 23 x 23 km^2 (at sub-satellite point). The GeoTROPE measurements and instrumentation are novel and innovative, but based on proven instrumental concepts and on the heritage from successful missions previously flown on LEO platforms.

Both instruments are operated 24 hours/day (except during S/C eclipse), requiring a dedicated data reception antenna for handling a continuous data stream (approx. 50 Mbit/s).

The mission concept will be realised by using the instruments mounted on a dedicated developed spacecraft, based on a modification of a commercial telecommunications platform with enhanced attitude and orbit control system to achieve the required pointing stability. For earth observation applications from an geostationary orbit accurate spacecraft pointing is required. So similar to Low Earth Orbit (LEO) missions like ENVISAT or METOP the attitude and orbit control system (AOCS) has to be equipped with star-tracker and gyros. But compared to LEO missions autonomy can be minimized due to the continuous contact to ground.

For the GEO-Mission a strong synergy with the Meteosat Third Generation (MTG) is given. For future meteorological applications advanced imagers and an additional Infrared Spectrometer are needed which require also an operation on a 3-axis stabilized spacecraft platform. Also similar configuration constraints like solar array configuration in combination with deep space view for thermal radiators have to be taken into account. Additional communality is given e.g. on mission aspects like orbit transfer and maintenance or environmental aspects like thermal and radiation environment.

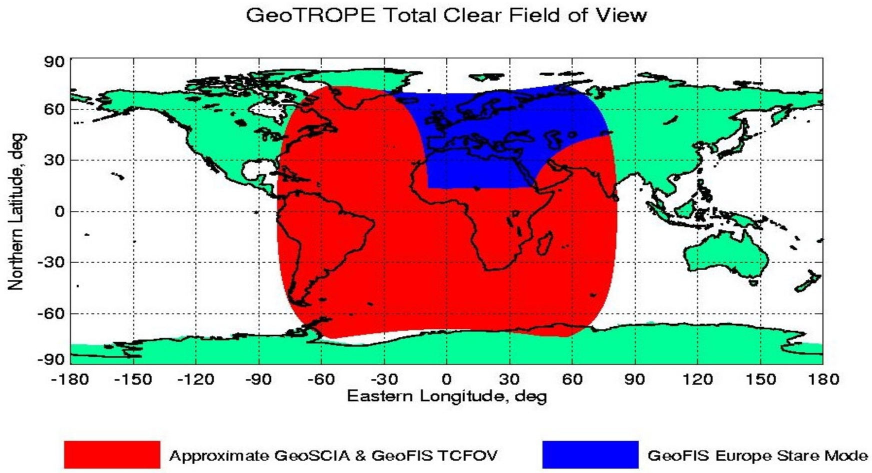

Figure 7.3.1-1. Earth coverage, in red the MTG Full Disk coverage as seen from GEO is shown, but based on actual Capacity requirements the coverage can be limited for Capacity to the blue area over Europe

7.3.2 GEO Payload

This section gives an outline of two instruments which are foreseen to perform the geostationary atmospheric chemistry mission. From the requirement discussion which is given for the UV-VIS-NIR and the IR Sounding complement, it can be derived that a scanning imaging spectrometer and a Fourier transform sounder are the instrument types which can fulfil the mission objectives best.

Common Payload Aspects

The requirements (R1 up to R5) from the work package 3100 are applicable for both instruments and are therefore discussed commonly here. Especially for the ground pixel size however, it needs to be checked whether dedicated requirements would be better.

R1: Coverage

The coverage requirement aiming mainly at Europe.

R 2. The FOV should be positioned over the Sahara for vicarious calibration purposes.

This can be achieved by an increased FOV of the instrument or by pointing. Here it is important to define the required frequency of such calibration. A first statement is that this has only to be done on a monthly basis. In that case we would recommend using the smaller FOV and using dedicated satellite pointing manoeuvre for this calibration. This leads to a smaller baffle, hence a compacter instrument.

R 3. The target requirement on IFOV is 5 km x 5 km at sub-satellite, corresponding to approximately 5 km x 10 km over Europe (latitude dependent). Threshold is 20x20km.

This requirement defines the pixel IFOV and the sample integration time. It has the largest influence on instrument scaling. However we understand that higher spatial resolution (smaller pixel sizes) have highest priority. We therefore applied 5x5km nadir pixel for the following assessments.

The threshold of 20 km x 20 km applies at sub-satellite point. So one order of magnitude is given for relaxation of this requirement. It is recommended to iterate this requirement and analyse the impact of this relaxation on instrument dimensions and design in the future study.

R 4. The instrument shall cover the FOV within 1 hour.

This is an important relaxation compared to MTG (30min.) especially in combination with the reduced coverage area.

R 5. The geolocation of the individual spatial pixels must be known with a precision of better than 10% - 30 % of the pixel.

Based on the threshold of 20 km x 20 km this requirement is similar to MTG (2 km - 6 km instead of 3 km) and considered as feasible.

The UV-VIS-NIR Sounder

The overall goal of the UV-VIS-NIR Sounder mission is to improve Air Quality (AQ) monitoring and forecasting in Europe by making synoptic measurements of the changing atmospheric composition of the troposphere at the relevant timescales (2 hours threshold, 30min. goal) and with the appropriate spatial resolution (10km over Europe).

The UV-VIS-NIR Sounder mission instrument profits from the heritage and experience gained with the existing instruments like SCIAMACHY, GOME and OMI, as well as from studies for example on EoGEO and on UVS for the ESA/Eumetsat MTG Mission as performed by EADS Astrium.

Requirements Discussion

Due to the topicality and strong similarity we performed the requirement discussion mainly by a comparison between the MTG-UVS and the new Capacity UV-VIS-NIR Mission requirements. But for the driving radiometric requirements dedicated simulations have been used for a simple instrument sizing assessment, which is only able to provide order of magnitude estimates.

Capacity demands more spectral coverage compared to the MTG UVS Mission. However, considering that the spectral resolution of the Capacity mission is reduced compared MTG, the influence on the data rate is limited and the lower spectral resolution helps to achieve a higher SNR, hence to limit the instrument size.

Conclusions on Requirement Assessment

Compared to the actual UVS mission requirements valid for the MTG Mission, a number of important relaxations have been identified. The combination of reduced earth coverage (concentrating on Europe), relaxed repeat time and relaxed spectral resolution, counterbalance the slightly higher spatial resolution and the larger spectral coverage.

Considering the UV-VIS-NIR mission only, the instrument would need a radiometric aperture of about 70mm, which is considerably less as so far assumed for the UVS instrumentation on MTG.

Additionally to the recent MTG UVS requirements, the implementation of a SWIR channel is specified as option. It is recommended to clearly quantify the added value of this channel to the operational mission, because from a technical point of view, adding this channel increases significantly the instruments complexity. In this case there are two areas to be mentioned:

(1) The detector technology of the needed SWIR detector is a lot more critical as for the UV-VIS-NIR range, especially considering the maturity of European technology. It is likely that available detector sizes, pixel sizes and shapes, are much more limited as for CCD or APS

technology. Additionally such detectors require cooling down to temperatures in the order of < 170K. This demands powerful cooling systems and the design of cryostats for the FPA.

(2) Considering the CAPACITY requirements on the SWIR channel, we calculated that this channel would drive the radiometric aperture of the instrument. We calculated 120mm instead of 70mm for UV, which is driving in the "visible" spectral range. It is recommended to asses if the added value by this channel justifies the larger system or if reduced performance, which can be provided by a 70mm system, may be acceptable.

Instrument Design Outline

With the current specification we would favour an east-west scanning imaging spectrometer with 4 spectrometers (UV, VIS, NIR and SWIR) similar to the Post-MSG concept as given in Figure 7.3.2-1, but considerably smaller due to the actual requirements. In terms of required detector technology, the UV-VIS and NIR channels can be covered by a dedicated CCD, which may be common for different bands, apart from the anti-reflection coating. The CCD detector is considered as mature technology, but has to be treated as a long lead item (LLI) in terms of the instrument development schedule. APS detectors may be investigated as alternative solution. If a SWIR channel is requested, this imposes higher constraints on the detector technology, size, the cryostat design and the cooling systems, which is preferably passive, but is likely to consume considerable resources in mass and volume.

The spectral coverage imposes also constraints on the telescope and polarisation requirements. For polarisation requirements different strategies are possible, designing an insensitive instrument, which is preferred especially with a limited spectral coverage, or an additional polarisation measuring system, which may be able to provide additional products, but at the expense of higher system cost and risk.

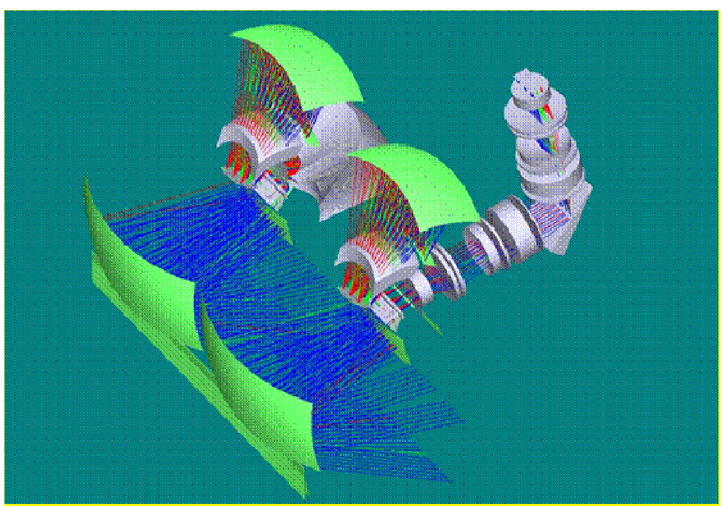

Figure 7.3.2-1. UVS optical design for Post-MSG mission Study. The system incorporates 4 spectrometers

Instrument Design Budget

For an instrument with the given coverage (limited to Europe) and repeat cycle, we would estimate a mass in the order of 100kg for an instrument without the SWIR band and with a simplified calibration concept, probably not full compliant with all requirements. Including the SWIR band and a polarisation measuring system (PMS), it is likely to rise to 150kg. This is however a simplified estimate, purely by comparison with the concepts of Post-MSG, MTG and GeoSCIA, mainly based on radiometric assessment. Reduced coverage requirements, longer repeat cycles in combination with different SNR specifications lead to considerably smaller budgets compared to Post MSG instrument. More detailed analysis taking all dedicated requirements into account may alter this numbers significantly.

Conclusions

We consider the requirements so far specified for the Geo UV-VIS-NIR Sounding Mission as complete and potentially leading to a reasonable instrument sizing. Some requirements on calibration, like radiometric accuracy, appear very demanding and may lead to discussion on cost and feasibility. Note that within the frame of this study we tried to concentrate the assessment more on sizing aspect. It is necessary to assess all requirements like calibration aspects in detail, which is indeed a complex matter and may be subject of a Phase A study.

In the performance specification document it is written that the instrument is meant to be insensitive to polarised light and alternatively the state of polarisation of incoming light shall be measured. There is however no dedicated requirement on polarisation sensitivity. Some other requirements (R6 to R9) demand the implementation of specific calibration hardware (e.g. sun diffusers), such requirements can not be quantified (apart from checking whether it is implemented). Those requirements maybe transformed into design recommendations, and are already partly covered by the radiometric and spectral accuracy requirements.

The analysis herein is based on the target requirement for the spatial resolution of 5 km x 5 km. This requirement is directly driving the size of the instrument telescope and so also of the instrument itself. As mentioned above applying the threshold of 20 km x 20 km results in a reduced instrument envelope and budgets. So a significant relaxation compared to the MTG-UVS is expected.

TIR Sounding Mission

Requirements and instrument concepts

In order to perform the instrument sizing, some key parameters are needed such as the four resolutions (spectral, spatial, temporal, radiometric).

The required spatial sampling of this mission is not so clearly specified in the documentation. Principally requirement R3 (5x5 km^2 goal, and 20x20 km^2 at nadir as threshold) is considered applicable for the Geo UV-VIS and the Geo TIR Missions. However a high spatial resolution is considered highest priority for the Geo UV-VIS mission, it is not clear if this applies also for the Geo TIR Mission.

For the TIR sounding mission we concluded that (in contrast to the UV-VIS Mission) a 5km nadir sampling would be too demanding for the instrument, so we started assessments with sampling of 10x10 km^2 nadir, this is the basis for all assessment about the TIR sounding instrument.

A very rough penalty score, considering the 4 resolutions and the scene extend has been performed. As this score gives a trend for the relative sizing wrt. MTG, it can bee seen that CAPACITY can be much more demanding or even relaxed (especially concerning data rate), depending on the desired spatial sampling.

A comparison of the spectral bands for MTG and CAPACITY shows that although for similar spectral range range, the spectral resolution is much more severe for the CAPACITY instrument.

An assessment of spectral parameters and resulting data rate of a dispersive spectrometer type of instrument operating in pushbroom mode is presented. For dispersive spectrometers, especially with the use of gratings, it is more convenient to work in microns/nanometers instead of wavenumbers. That's why the units are not in wavenumbers.

For each channel the number of spatial samples is between 800 and 6400 per spectral Band. This would require large detector arrays with many pixels and a number of spectrometers, probably with a number larger than the number of spectral bands. A dispersive instrument operating with such a lot of spectrometers is considered as practically too complex. We conclude that a Fourier Transform Spectrometer would result in a more simple design approach for the same sizing requirements.

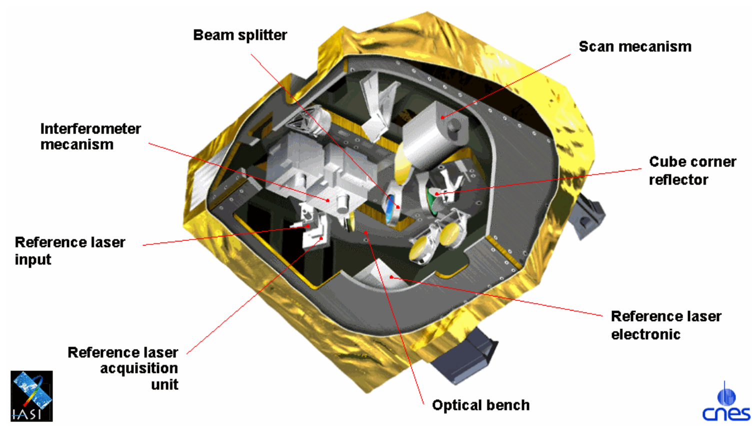

Figure 7.3.2-2. The GeoFIS principal components (IASI, courtesy CNES).

<u>Conclusions on Requirement Comparison and first concept trends</u>

Compared to MTG infrared sounder, the similar spectral range with much higher spectral resolution and combined with higher S/N requirements results in a rather challenging instrument when selecting a dispersive sounding instrument type. For a 10x10 km² spatial sampling, the size is expected to be even higher compared MTG version of IRS, due to a larger number of spectrometers required.

From the common requirements we understand, that 5km at nadir is the goal and 20km at nadir is the threshold. From a first radiometric analysis on FTS we concluded that the 5km spatial sampling would not lead to a reasonable instrument size. Only with a 20km nadir sampling, the instrument aperture may be in a reasonable order of about 200mm to meet the SNR requirements.

For a Fourier transform type of spectrometer, such a pupil can not be handled reasonably by a Michelson interferometer type of spectrometer. When using such a spectrometer type, a pupil reduction is needed, e.g. by means of an afocal telescope. Such a telescope magnifies the field angle by the same factor as the pupil is reduced. Since there is a performance limitation in the field of the interferometer of a very few degrees, a split of the Earth N/S scene has to be made in several different stare positions (in E/W anyhow this split is needed), requiring as a consequence a 2 axis scan mirror at the fore optics.

Taking as starting point the MTG IRS and a spatial sampling of 10 km x 10 km, then the interface data will have the order of magnitude as follows:

Mass: roughly 250 kg

Power: Approximately 250 W, including active cooler

Data Rate: ca. 15 Mbit/s if FFT processing and spectral resampling is performed on board

Volume: Optics Module: 1100 x 1600 x 800 mm³

These data are results of a first rough estimation and need to be confirmed in further iterations. The analysis herein is based on a resolution of 10 km x 10 km. The target requirement for the spatial resolution is 5 km x 5 km, the threshold 20 km x 20 km. This requirement is directly driving the size of the instrument telescope and so also of the instrument itself. As mentioned above applying the threshold results in a reduced instrument envelope and budgets.

7.3.3 Geostationary platform aspects

Herein this short assessment no detailed analysis of the satellite design can be derived but a first outline can be given, especially by comparison with the MTG study. Based on the requirements of both, the CAPACITY and the MTG mission, these operational observation concepts can be realised only on 3-axis stabilized platforms. Up to now no 3-axis stabilized platform is developed and launched for earth observation applications in Europe.

So for the first time in Europe it is planned to develop such a platform within the MTG project. But for programmatic reasons the trend of the actual MTG study is to reduce the satellite sizing by using dedicated satellites for each instrument-mission. In this case the platform design driving instrument is the MTG-IR-sounder.

Due to the fact that the dimensions of the CAPACITY-IR-sounder are similar to the MTG-IR-sounder but with the UV-VIS-NIR sounder an additional instrument has to be accommodated it is expected that the needed capabilities of the CAPACITY spacecraft-platform in form of payload mass and power are higher. On the other side it is not expected that the parallel development of two different geostationary platforms is problematic. So it is recommended to take the re-usage of the MTG 3-axis stabilized platform as much as useable for CAPACITY and not to reduce the CAPACITY payload to the capabilities of the MTG platform.

A specific challenge is the high pointing performance needed from the geostationary orbit. It is expected that very detailed analysis of the measurement principles by simulations are needed to derive the correct pointing requirements. Concerns are not only the requirement values but also which kind of pointing accuracy is needed. It is recommended to start with the definition of the needed pointing stability, may be without any requirement on the absolute pointing accuracy.

For meteorological applications earth image data are corrected by data processing on ground. Image processing methods based on so called ground control points are applied. It is recommended to investigate the feasibility to use the same or similar methods also for the sounding applications proposed for the CAPACITY geostationary mission.

7.4 LEO Applications

7.4.1 Mission and Systems Concepts

The LEO-Mission is driven by the need of additional global observations of the atmosphere, complementary to meteorological data obtained by the ESA/EUMETSAT METOP program. Based on results of the CAPACITY study two main aspects are yielding two optional mission scenarios for operations of satellites in a low earth orbit (LEO):

- **Limb option:** METOP data relevant for Capacity are obtained by total column nadir measurements. A vertical resolution is estimated by model assumptions based on vertical pressure profiles derived from measuring the spectral broadening (usually O2). For most constituents of interest this is not sufficient as they appear in dedicated layers. So Capacity is driven by requirements on complementary observations using Limb measurements with improved vertical resolution compared to ENVISAT MIPAS, SCIAMACHY and GOMOS data.
- **Nadir option:** With a single sun-synchronous LEO-satellite it is not feasible to measure the impact of diurnal variations on the observations. So by an additional Nadir-mission complementary to METOP the diurnal variation can be observed. Also the local observation frequency required for protocol monitoring observation of the air-quality can be improved.

For Capacity the LEO observations are mainly driven by products needed for monitoring of the Ozone Layer and Climate.

The LEO-Limb Option

A first mission concept similar to the Limb option discussed herein was already proposed in the Atmospheric Chemistry Explorer mission study (ACECHEM, ECM2 Pre-Phase A Study of Candidate Earth Explorer Core Missions). ACECHEM is to measure and to understand the human impact on the chemistry and composition of the atmosphere with the focus on Stratospheric ozone recovery, Tropospheric cleansing, Pollutant export, Aircraft impacts and Biomass burning.

The atmosphere is observed in limb sounding geometry. The volume densities of dedicated species are determined by measuring the absolute power densities of specific spectral bands. A height resolution is achieved by either vertically scanning the antenna/telescope or by receiving the radiation with several sensors in parallel.

The Limb option shall be operated in a tandem orbit with METOP to ensure spatial and temporal simultaneity of the measurements by limb sounding measurements of Sentinel and the nadir measurements of METOP. The Capacity Limb mission, also as investigated in ACECHEM, consists of two optional limb monitoring payloads, which are the AMIPAS and MASTER. These instrument options shall be developed exclusively, so further trade-off analyses have to be performed in a future study for a selection of the payload. For both options the instruments are monitoring by limb viewing the air volume, observed simultaneously by the METOP payloads.

In contradiction to Capacity for the ACECHEM mission both instruments are baseline. A rather classical satellite design has been elaborated, taking into account the sun-synchronous morning orbit at 820 km altitude. The mechanical satellite configuration is mainly driven by the specific accommodation requirements of the AMIPAS and MASTER instruments.

The Capacity and ACECHEM data rate of 4 Mbps and data volume of 24 Gbit per orbit are mainly driven by AMIPAS. In contradiction to the GEO-Mission no continuous contact to the groundstation is given. So all housekeeping data generated by the platform/instruments as well as all instrument measurement data have to be stored on-board in a Mass Memory Module (MMM) for later downlink to the ground-station.

The LEO-Nadir Option

A first definition of the LEO Nadir option is also discussed herein the CAPACITY study. Alternative Orbits with local measurement time different to METOP are taken into account. The actual observation requirements will lead to an advanced SCIAMACHY instrument using the improved 2-D detector technology similar to OMI or GOME-2.

So scenarios with single or multiple LEO Nadir satellites and in combination with the parallel operating METOP mission the diurnal variation in the atmosphere can be observed by higher observation frequency of products obtained by Gome-2 and IASI.

7.4.2 The LEO payload

The Limb IR Sounder

In Chapter 6 it was proposed to use for the Capacity LEO mission the AMIPAS instrument from the ACECHEM study.

AMIPAS Architecture

The optics module comprises a 70mm aperture in the front optics which includes pointing mirror and afocal telescope with magnification factor of 2. The following spectrometer is based on a small tilt and shear compensated michelson interferometer, with a small mechanical reflector travel of +/- 6.5 mm, using a lubrication free reliable mechanism. A simple relay optics transfers the interfered beams through a cold optics compartment to the two 15x15 pixels detectors, one for each band, housed in a common focal plane assembly and cooled to around 55 K by a doublet of pulse tube coolers. Instrument line of sight pointing to a calibration blackbody and cold space allows radiometric calibration.

The signal electronics comprises near electronics close to the detector, video processing and digital signal processing functions as well as wavelet transformation and formatting functions. The control and functional electronics allow the instrument command and control.

Comparison Capacity spec – AMIPAS performance

A comparison has been performed between

- the main capacity requirements (extracted from a specification “part 7: Mission level Requirements” received from WJ Reburn 1.4.05 and
- the AMIPAS performances documented in the Detailed design description of AMIPAS, ref. AMIPAS-ASG-TN-30, Oct. 2003

In conclusion the AMIPAS matches very well into the capacity specifications, with a small exception of radiometric resolution. This can be achieved by enlargement of the telescope radiometric entrance pupil, with associated increase of optics speed and degradation of point spread function.

In addition, it has to be noted, that a dark current noise performance of the detectors is assumed which is 10 times better than existing European technology can provide. Therefore considerable development effort has to be undertaken for improvement of the technology rather soon.

AMIPAS Interface Data

The following interface data for AMIPAS have been estimated:

Mass: 170 kg (without limb cloud imager)

Power: Approximately 180 W

Data Rate: 4 Mbps after lossless compression

Volume:

Optics Module: 920 x 640 x 230 mm³

Electronic Module: 945 x 718 x 220 mm³

The Limb mm Sounder

The Millimetre-wave Acquistions for Stratosphere/Troposphere Exchange Research instrument (MASTER) will measure molecular thermal emission spectra at millimeter and submillimeter wavelengths. Constituent profiles will be derived by scanning the atmospheric limb in vertical direction.

The instrument consists of a number of functional blocks as illustrated in Figure 7.4.2-2. The incoming radiation is received by a large scan antenna and distributed into 4 or 5 discrete spectral bands where they are individually down converted and amplified by a set of heteorodyne radiometers. Their output signals are multiplexed and passed to a set of spectrometers measuring the spectral power density across each band. For calibrating the power measurements the instrument will look in regular intervals to deep space and a carefully temperature controlled hot target.

The main subassemblies of the instrument are:

- A 2 m x 1 m offset Cassegrain antenna, driven by a dedicated scan mechanism with a subsequent optical network for beam distribution
- A dedicated calibration assembly
- A set of heteorodyne radiometer frontends for down conversion of the mm-wave signals to an IF in the range of 15 - 20 GHz; the frontend mixers have to be cooled down to 80K and to 240K respectively
- An IF distribution network for apportioning the spectral bands to the spectrometer needs
- A set of acousto-optical or autocorrelation spectrometers covering a total spectral range of 25 - 30 GHz with a resolution of at least 50 MHz

An instrument control unit for command and control and a data processing unit for data compression and formattin

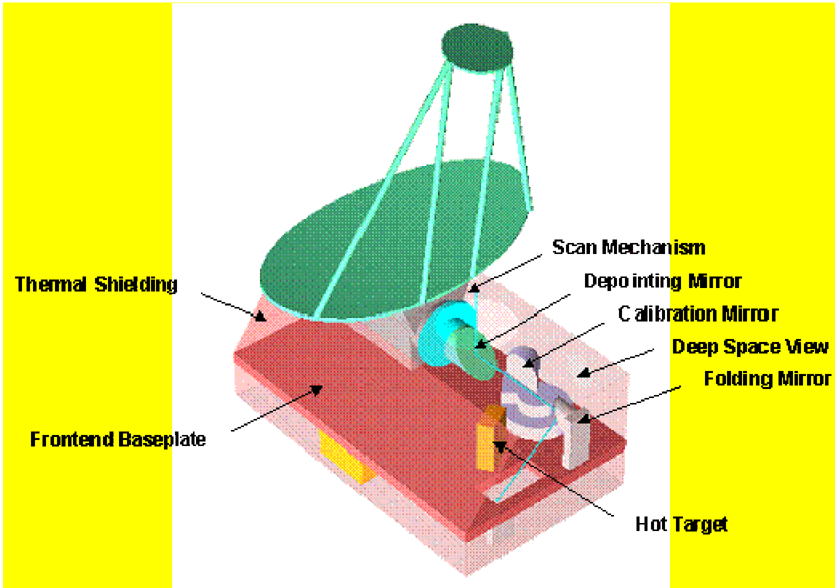

Figure 7.4.2-1. The Master instrument

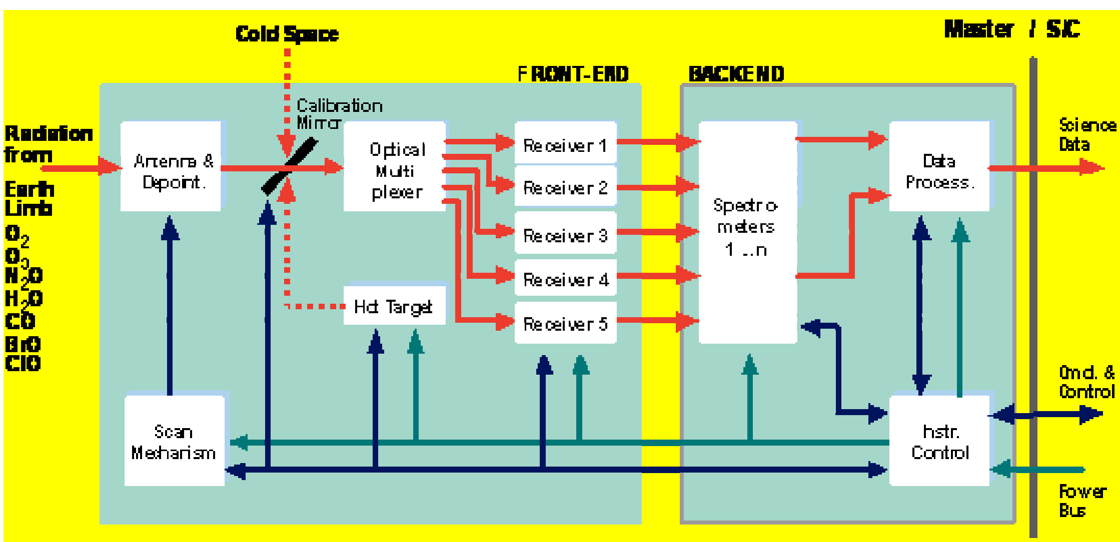

Figure 7.4.2-2. Master Functional Blocks

The Nadir-UV-VIS-NIR Sounder

The UV-VIS-NIR instrument profits from the heritage and experience gained with the existing instruments like SCIAMACHY, GOME and OMI. The main difference from the GeoSCIA mission is the lower repeat cycle which is here typically below one day. This instrument can record total ozone and other atmospheric parameters related to ozone chemistry and climate, and can measure key air quality components and aerosol characteristics.

Requirements Discussion

The following assessments are based on the preliminary SRON document (SRON-EOS/RP/-5-x). This document defines the instrument spatial sampling and swath, however it does not specify where the pixel size shall be met (nadir or edge of swath), and for which orbit (respectively for which revisit time) this applies. Therefore the following assumptions are taken: 10x10km nadir, 820km (Metop orbit). It is import to notice that for constant detector pixel sizes, the related ground pixel size increases drastically towards the edge of the swath by geometrical projection.

Instrument Design Outline

Like SCIAMACHY (see Figure 7.4.2-3) this instrument can either operate as a whisk-broom scan concept, scanning one or more lines on ground. This class of instrument requires a scanner and a larger aperture compared to a push-broom scanner, but can offer a large swath and calibration views with a simple optical concept.

Alternatively the instrument can work in a push-broom fashion like OMI, which reduces significantly the required instrument aperture, but puts limitations on the optic, which has to cover a large field. Advantage is that no scan mechanism is needed, but most likely additional mechanism for calibration purposes.

Instrument Design Budget

As a first idea, the instrument parameters can be assumed in the range between OMI (65kg, 70W) up to SCIAMACHY (200kg, 150W), where the lower limit of OMI is rather unlikely to be met, because the required spectral range is different and likely to demand 3 instead of 2 spectrometer (OMI).

Note that this is not based on a radiometric assessment, which may lead to very different results!

Conclusions

The above mentioned budgets are established in comparison with existing instruments. Due to the limited EADS Astrium scope in this study were not yet able to establish a performance model based on the given requirements. We were however able to review the consistency and completeness of the requirements. We consider the specifications as comprehensive and consistent, apart from some comments we made already: E.g. it needs clear specification where the required spatial pixel size applies (nadir or edge of swath), furthermore orbit or revisit time should be specified. Many requirements relating to calibration aspect appear very demanding, we would expect later discussion on feasibility and cost.

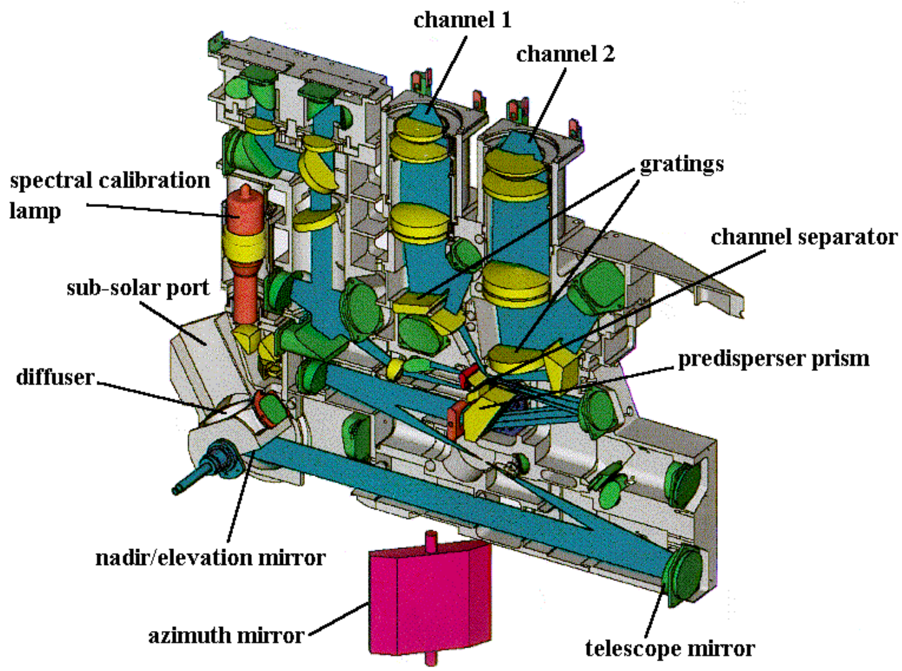

Figure 7.4.2-3. Overview over the Sciamachy imaging spectrometer

7.4.3 The Low Earth Orbit Payload Aspects

In contradiction to the geostationary orbit a strong heritage of the 3-axis stabilized platform is given for low earth orbits. Many different designs are showing the application specific solutions like for the operating ENVISAT or future METOP spacecrafts.

Nevertheless mission specific aspects have to be taken into account. Herein the Capacity mission it is expected that the amount and rates of measurement data to be handled and stored on-board the spacecraft will drive the design.

Also for the Limb mission it is required to improve the vertical resolution of the instruments. So the need of higher platform pointing accuracy is given. Based on an 800 km orbit altitude the distance from satellite to the horizon is 3293 km. The needed pointing accuracy is similar to the geostationary platform, if this distance combined with the required vertical resolution of 2 km of the Leo-Limb-Mission is compared to the Geo-Nadir-Mission with 20 km spatial resolution.

But generally no critical platform aspect is identified to be taken into account in this early Capacity assessment.

7.5 Summary and Conclusions

In the context of the ESA CAPACITY study on the definition of future operational atmospheric chemistry missions the results of work package WP 3300 are documented in this chapter.

Based on the inputs of Chapter 5 (WP 3100) for geostationary and of Chapter 6 (WP 3200) for low earth orbit applications first assessments to show feasibility are performed. Most of the defined mission requirements are reviewed and iterated with WP3100 and WP 3200. They are also analysed by showing similarity to already existing investigations, mainly derived from the MTG, GeoTrope and Acechem studies. For specific aspects first mathematical simulations are performed to outline e.g. radiometric instrument performance.

Due to the nature of an operational mission already the inputs to WP 3300 have taken existing missions and instruments into account. As result none of the assessed instrument concepts required for the geostationary or low earth orbit missions is completely new, so based on the heritage of already existing missions feasibility is implicitly given. But improvements are needed, e.g. to achieve in the LEO-Limb mission higher vertical resolution. Especially due to the further development of performance relevant items, e.g. large infrared detectors and the needed cooling equipment, major performance improvements are expected. In future studies more detailed analysis are needed to show the full technical impact of the required modifications in combination with the predicted technologies.

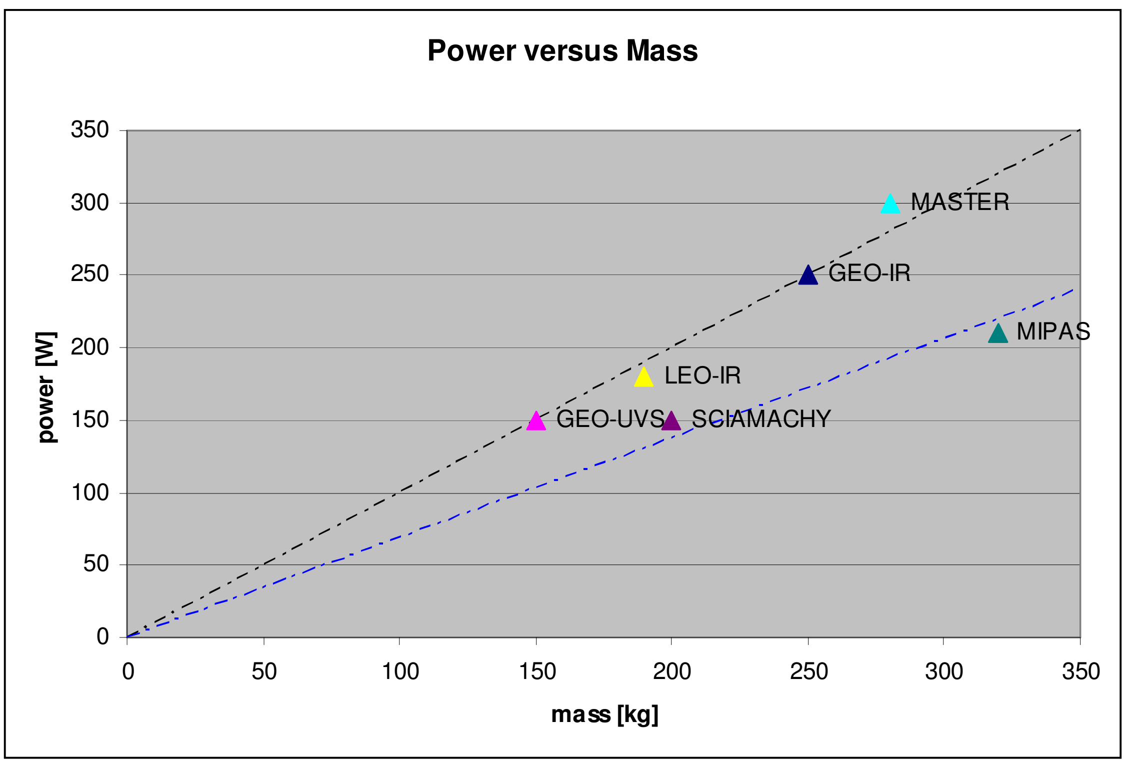

Figure 7.5.3-1. Instrument Power and Mass budgets.

Based on the preliminary conceptual instrument designs resulting budgets for power and mass are compared in Figure 7.5.3-1. Additional budget information of SCIAMACHY and MIPAS on ENVISAT are given to show reference values of existing instruments. This figure gives a qualitative indication for the needed development effort of the different instrument designs. But the conclusions are preliminary, e.g. presently MASTER seems to be the most driving instrument. It is expected that further iterations on the instrument requirements may change this figure. Nevertheless the UV-VIS-NIR concept needs the lowest development effort combined with the highest heritage, see also GOME-1/2, SCIAMACHY and OMI.

Herein this work package an additional assessment is performed on mission design alternatives to the conventional geostationary and low earth orbit options. Principally a constellation of 3 satellites in low earth orbits is an interesting compromise between the GEO and LEO applications, especially if for all applications the same set of instruments can be used. Particularly if additional requirements on the mission reliability are given, as expected for an operational mission, such a constellation may have also cost-advantages.

But it has to be mentioned that the most driving revisit time requirements of 0.5 to 2 hours of Nadir-measurements for air-quality applications are not fulfilled by a sun-synchronous 3 satellite constellation. Also a strong impact of the protons radiation, which is increasing with altitude, is given on satellite and instrument design, lifetime and costs. So a reasonable rise of the orbit altitude is very limited seems not to be well adapted for an operational mission. The situation strongly improves for low earth orbits with lower inclination. An example shows a feasible revisit time below 2 hours for 894 km orbit altitude. But similar to the geostationary this orbit has not been used up to now for earth observation in Europe. Therefore it is strongly recommended to study such a constellation in detail taking all measurement and technical aspects into account. As examples it has to be mentioned that the changing local time of the spacecraft has strong impact on the evaluation of the observation and also on technical aspects like power or thermal spacecraft system.

Observations with high vertical resolution which are not given by already planned missions like METOP are driving the need for additional Limb-measurements performed in the low earth orbit. It has to be mentioned that different instruments are needed dedicated for Nadir and Limb observations to cover all applications discussed for CAPACITY.

The resulting conclusion is that the actual Geo-mission and Leo-mission requirements are further complementary. A combined mission based on a constellation of 3 satellites in a sun-synchronous or an orbit with low inclination may be a compromise. So if it is not intended to develop both, a dedicated GEO- and a dedicated LEO-mission, further more detailed trade-off analysis of potential implementation scenarios are recommended. Such an analysis has to balance the needed development effort against the observation performance and the priority of the different mission objectives.

8 Evaluation of Critical Ground Segment Issues

8.1 Introduction

The purpose of this chapter is to present a preliminary description of the integrated Capacity ground segment taking into account the combinations of missions.

8.2 Main assumptions

The main working assumptions for the Capacity Ground Segment (CGS) are:

- The CGS will be implemented as a development of the current multi-mission ground segment.
- The CGS will be based on a modular architecture that reuses available standards and proven technologies.
- The CGS will be based on a distributed processing approach using existing centre of expertise that already implement the required models.
- The CGS will be completed by the "service segment" needed for providing customised services.
- This approach is similar to existing operation system like METEOSAT and MSG
- This approach is similar to the one adopted for Sentinel 1, Sentinel 2 and Sentinel 3.
- Services provided by the entities managing the models will be fully operational at the time the Capacity Ground Segment is available.
- LEO mission requirements are compatible with a dump strategy of a single dump per orbit.

LEO and GEO instruments and missions are systematic : the users cannot requests specific instrument mode and sensing, the instrument mode and sensing are defined from mission requirements and performed systematically.

8.3 Main functions of the capacity ground segment

8.3.1 Perimeter of the CGS and functional breakdown

The breakdown of the Capacity segment into other segments and functions is:

- The Capacity space segment (including the spacecraft(s) and the launch vehicle)
- The Capacity ground segment
    - data acquisition at receiving stations,
    - interface to direct access stations,
    - data processing (level0, 1, 2)
    - data archiving and retrieval, local catalogue,
    - data assimilation into models,
    - eventually, generation of end products,
    - monitor the instrument performances,
    - product quality assurance,
    - control and command for the mission satellite,
    - mission planning (data download, stations operations, production scheduling, dissemination scheduling)
- The service segment

  - o user services including catalogue, order handling, user handling, user interface and support.
  - o data distribution to end user,
- The Capacity collect segment
    - o to collect other data from other cooperative space missions,
    - o to collect other data from ground base sensors network (airborne sensors, etc)
    - o to collect auxiliary and ancillary data

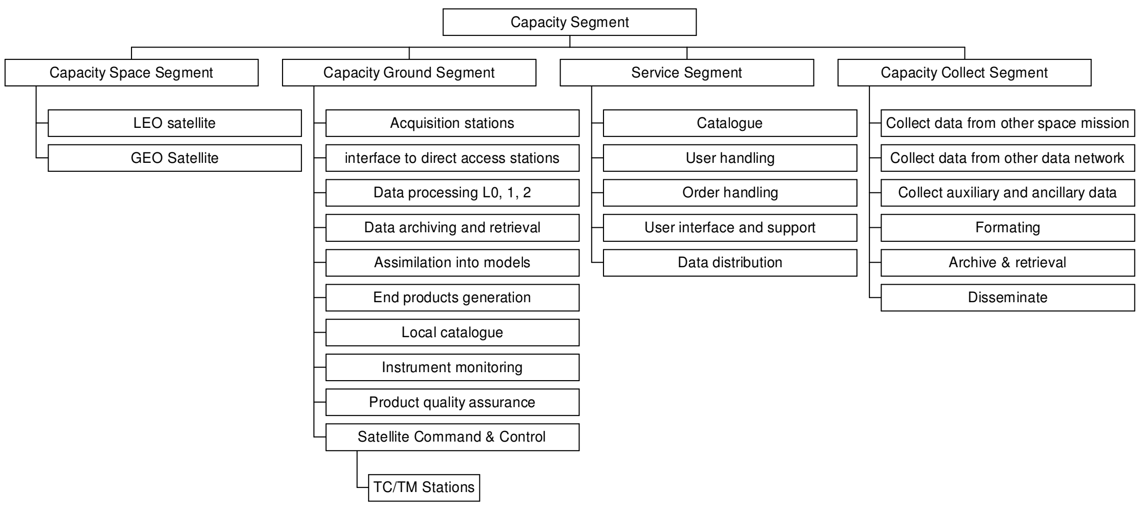

Figure 8.1 Breakdown of the capacity segment.

Driving requirements

According to the current requirements identified in previous paragraph and to the needs of an operational system, the main drivers and specificities for the CGS are:

- the NRT requirements for the delivery of Air Quality basic products (< 2 h TBC)
  - o this requirement applies to the B1 theme and could be limited to an area of interest (e.g Europe)
  - o B2 theme requires, for instance, a delivery of service each morning for the coming day. The measurements of day “D” could be processed during the night and delivered the morning of day “D+1”. No NRT requirement is then associated to B2.
- the high availability required for an operational system will induce the need of redundancy
  - o Sentinels 1, 2 and 3 requirements identify a product delivery availability higher than of 90 % leading to a ground segment availability close to 100 %.
- the robustness and reliability will require autonomous/validated processing models.
- the management of sentinel 4 in a geostationary orbit will require specific measure and Flight Dynamic System with respect to “classical” LEO orbit, but ARTEMIS and METEOSAT experience could be use efficiently.

The NRT requirement is less a driver for a geostationary spacecraft (sentinel 4), but has several impacts when dealing with a Low Earth Orbiting spacecraft (Sentinel 5). This impact is clearly limited if the requirement is applicable to Europe only because simultaneous acquisition and downlink could be organised, for instance.

A global NRT requirement will require the use of Svalbard as the single ground station, several receiving ground stations or the use of geostationary relay satellite (like ARTEMIS).

The current requirements of Sentinel 1, Sentinel 2 and Sentinel 3 ask for the use of a single ground station. Consequently, each sentinel selects Svalbard as the ground station, thus leading to a potential overcrowded situation of the receiving ground station.

The first recommendations would then be:

- increase the capacity of Svalbard ground station in order to be able to manage such a float of spacecraft,
- optimise the local time of each mission taking into account the local time of the other missions sharing the Svalbard receiving ground station,
- assess the additional cost induced by the use of several receiving ground stations,
- confirm the global or local applicability of the NRT requirement.

This NRT requirement does not impact only the downlink strategy, but also the architecture and infrastructure of the ground segment.

External interfaces

The following figure illustrates the interactions between the capacity segment components and identifies the main interfaces between these elements.

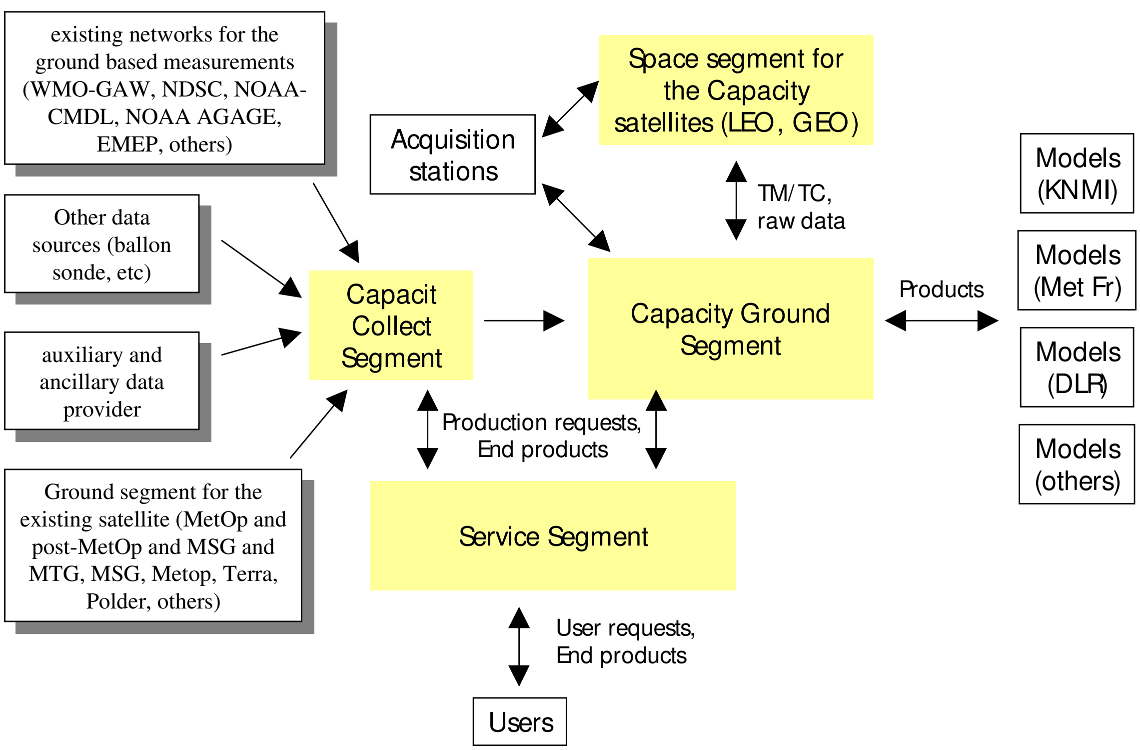

Figure 8.2 Interactions between Capacity segment components.

In the above figure, the "service segment" and the "capacity collect segment" are segments that shall have multi-mission capabilities :

The “service segment” shall provide a user interface for order deposit that is mission independent. The “service segment” will then breakdown the order into productions requests sent to the adequate ground segment, possibly using the “capacity collect segment” to interface with missions other than the Capacity mission.

The “service segment” shall provide also production dissemination services capable to route to the destination user end products according to the parameters of the original request and this whatever the requested end product.

The “capacity collect segment” shall provide a unique and standard means to interface existing ground segments, data networks and data sources for auxiliary and ancillary data.

The “Capacity ground segment” is not multi-mission (meaning that it cannot be switched by a change of configuration to support another mission) but it shall be developed using generic components (multi-mission components, e.g. for archive, catalogue, etc.), generic interfaces and standards.

The “Capacity ground segment” will interface the different existing models for data assimilation. Possibly new models may be needed and shall be developed. The interface between the “Capacity ground segment” and the different models shall also be generic in order to facilitate future integrations.

The “Capacity ground segment” could have its own acquisition stations or could also use existing stations : e.g. typically existing Svalbard acquisition stations for the LEO capacity satellite.

Products tree

Ground segments are typically depicted using functions or components and interfaces. But another way to depict ground segments is to describe the different transformation of products and their inter-dependencies.

The capacity study has been conducted by asking to scientists “what are the physical measurement that are needed in order to fulfil the data requirements ?”. The answer being lists of gases for which atmospheric concentrations measurement are requested and per gas, the specification of the spatial resolution, altitude range, revisit time and accuracy needed.

However, for the ground segment, the questions are more asked in terms of :

- What are the transformation needed (processing) to obtain these gas atmospheric concentrations from the instrument raw data ?
- What are the data (auxiliary and ancillary) needed to support these transformations ?
- What are the products requested by the end users : end products ? (e.g. what are the(s) user end product(s) needed for air quality forecast ?)
- What are the transformation needed (processing) to obtain end products from the gas atmospheric concentrations ?

Therefore a complete product tree showing all the transformation of data from the raw data, to the gas atmospheric concentrations, the input products for the models, the end products shall be drawn, showing interdependencies for products generation and relation to the auxiliary and ancillary data.

At this stage of the Capacity study, this product tree need to be completed in further phase study. It is nevertheless mandatory for assessing the amount of data to be archived, the data throughput in the system and the product generation timelines at all the steps of the processing. This is particularly relevant to this study as the data assimilation models are distributed over Europe.

As an example, air quality forecast rely heavily on the combination of ground based network, air quality models and satellite data, therefore, the product tree shall identify the ground based network products (associated data source shall be identified too) and the interdependency for processing shall appear in the product tree. In turn, this will have an impact on the timelines for the final product availability.

But in addition, attention shall be given to the area coverage, spatial resolution, vertical range, accuracy and age (with respect to the satellite data) of the ground based network products : these conditions must be satisfied in order that the multiple data sources are useful for product generation.

Another example is the need to compute precise GEO attitude before processing instrument measurements due to the required spatial resolution.

When drawing this product tree, one shall take into account the gas atmospheric concentrations for which requirements are effectively meet. Some branches of the product tree may well be not useful as the products generated may not fulfil the data requirements.

Topology for the capacity ground segment

The GEO satellite requires colocated TM/TC and data acquisition antenna close to the "capacity ground segment" central site in Europe.

The LEO satellite requires colocated TM/TC and data acquisition antenna at high latitude in order to achieve visibility over all orbits. The forwarding of data to the "capacity ground segment" central site could be done as for EPS (ground segment for Metop) : use of a satellite link (4 Mbps) between Svalbard and Europe, the raw data being cut-off in data packet, oldest downlinked data being send first.

Alternatively, as an optic fibre link (34 Mbps) will be soon available between Svalbard and Norway, it could be used in conjunction with terrestrial lines (ISDN) to get the data to the "capacity ground segment" central site.

Both solution are technically feasible, to-day, they do not present risks.

The LEO acquisition station at Svalbard could also be used to acquire systematically data from complementary mission. This will require coordination with the associated ground segment (e.g. to allow the satellite to perform 2 dumps in some orbits).

Alternatively, the "Capacity collect segment" could be used to get directly the needed products from the associated ground segment.

The compliance of the end to end timeline requirements (e.g. 2 hours for Air quality monitoring, 6 hours or 12 hours for the other applications) is more dependent of the product tree and dissemination means (to models and users) :

- List of successive transformation to be performed,
- Data needed for these transformation, it could mean waiting some auxiliary data or products generated by ground segments from other satellite,
- Link to/from the data assimilation models, assuming the processing will be available when the data are provided.
- Processing time required by the models,
- Dissemination link to users : ftp server, DVBS-RCS link.

At this stage of the Capacity study, no figure can be provided, but it is believed that the product tree and dissemination means (to models and users) are the major contributors to the end to end timelines.

Generic components
The definition of generic components could be achieved via standards that are either international standards or industry standards. Examples of these standards are the Open Archival Information System (OAIS), web services (SOAP, XML), C2C (customer to customer), OpenGIS (with WMS, WFS and WCS standards), EO GRID (Earth Observation, LCG2 middleware, etc. As a possible example, Grid could be used to access the models from the "Capacity ground segment".

8.4 Implication of combined missions on the ground segment

One of the outcome of Chapter 5 (WP 2300) is the need of multiple satellites system to fulfil the operational atmospheric chemistry requirements. However, Chapter 7 (WP 3300) has concluded that combined mission are not useful.

8.4.1 Impacts of multiple-elements atmospheric chemistry GMES missions

The main impacts are identified at the following levels:

- At data processing level
  - Products from GEO sentinel can be used as ancillary data for data processing.
- At product quality control and calibration/validation levels
  - Data from GEO sentinel and LEO sentinel can be compared and cross-checked to assess product quality and for calibration/validation activities.

8.4.2 Impacts of co-operation with additional cooperative missions

As highlighted during the study, the operational atmospheric chemistry will rely on future sentinels spacecraft and on existing or currently planned spacecraft such as MetOp, post-EPS and NPOESS. Cooperation between the GMES missions (the so-called Sentinels) and these cooperative missions will also impact the ground segment :

- at acquisition level : acquisition could be done via the Svalbard station (with adequate management of the satellite visibility and station sharing) or via the "Capacity collect segment". Additionally, the Svalbard station could be used as a back-up station for the cooperative missions (e.g. for orbits without visibility or in case of unavailability of the nominal acquisition station).
- At ground segment planning level : for acquisition and dissemination activities. In addition, the content of the downlink shall be agreed by both missions.
- At processing level : product tree.

8.5 Preliminary decomposition of the ground segment into functional elements

8.5.1 Identification of the high-level elements of the ground segment

Starting from the perimeter of the CGS defined in section 8.3.1, the functions could be detailed:

- Control and commanding of the space segment,
- Observation data acquisition,
- Other data collection from ground based measurement networks and ground segment from existing satellite,
- Data formatting, quality checking, archiving and dissemination to processing centres,

- Basic products processing (using distributed processing centres (TM3/KNMI, 3D NCAR-ROSE/DLR, CHIMERE/CNRS, IMAGE/CNRS, MOCAGE/Météo France, satellite data assimilation/ KNMI and Météo France, etc.) and possible other models (in order to service the 9 user communities)).
- Basic products collection from processing centres, archiving and dissemination to end users (9 communities).

A security function could be added to the previous one in order to comply with one of the key requirement of the GMES system.

Figure 8.3 identifies these main functions and their links for the more complex case where a lot of "external" data (in-situ, ancillary …) are required. It should be noted that, in this case, the NRT requirement of 2-3 h could be difficult to meet.

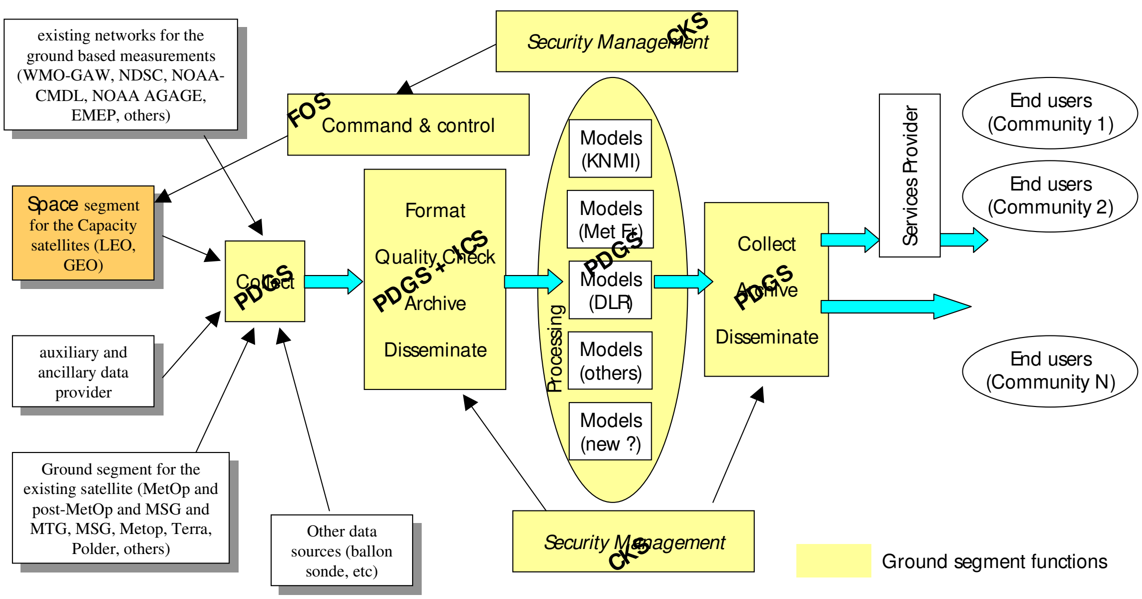

Figure 8.3: Functions and Allocation of the ground segment

Then, following one of our working assumption stating that the ground segment should be built on existing facilities, the CGS architecture could be split into 2 main entities interfacing with 2 supporting elements:

- the FOS "Flight Operation Segment" managing all satellite(s) monitoring and controls. It contains the control station which is able to exchange TM/TC with the SC and the control centre which is able to monitor TM and to prepare TC.
- the PDGS "Payload Data Ground Segment" ensuring the reception of all the observation data down-linked by the spacecraft, as well as other data, processing, archiving and distributing the data and associated basic products. The archive includes the long-term archive essential in the GMES context

  Two supporting elements interfacing with both of these elements:

- the ICS "Instrument Calibration Segment" managing all validation and quality aspects.
- the CKS "Cipher Keys Segment" generating and providing to the FOS and PDGS all the Cipher Keys necessary for security concept.

The FOS and the PDGS are independent, except for the observation plans and for the ICS/CKS.

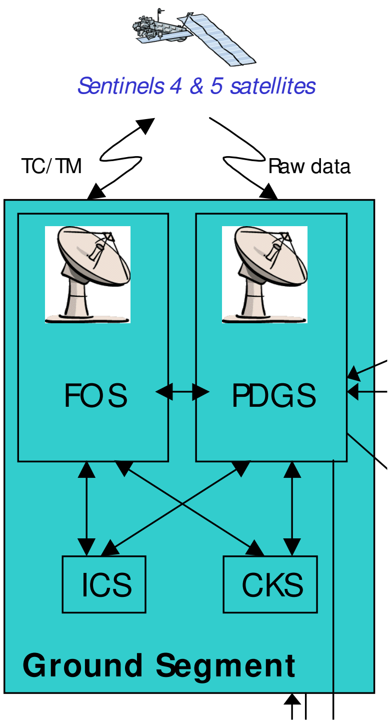

Figure 8.4: Identification of the ground segment high-level elements

8.5.2 Flight Operation Segment functions

The main functions of the FOS are:

- reception of telemetry data from the Space Segment,
- reception of the preplanning of the payload,
- planning of the platform, w.r.t its orbit and housekeeping,
- commanding of the Space Segment,

The ground systems elements included in the Flight Operations Segment in order to fulfil these functions would be:

- The Operations Control Centre including:
  - the Flight Control System for monitoring and control of the satellite,
  - the Operator Display System,
  - the Mission Planning and Scheduling System,
  - the Flight Dynamics System,
  - the On-Board Software Maintenance System,

  - the Performance Analysis System,
  - the Operations Preparation System,
  - the Spacecraft Simulator,
  - the Network Operations Centre.
- The Ground Station Network consisting of the stations for receiving telemetry and sending telecommands in S-Band.
- The Ground Communications Network providing the communications infrastructure connecting these ground system elements.

The main FOS interfaces are:

- the satellite for TM/TC/ranging,
- the PDGS for observation plans and instrument quality statuses,
- the ICS for calibration data,
- the CKS for cipher keys needed by TC authentication.

8.5.3 Payload Data Ground Segment functions

The main functions of the PDGS are:

- pre-planning of the payload (if needed) and planning of the processing chain,
- data processing (including generic lower level processing as well as dedicated processing for selected basic products (in distributed processing facilities)),
- centralised archiving (long-term and on-line),
- distribution of basic products and lower level data (if needed).

The PDGS infrastructure also includes

- The gateways for collecting external data (other satellites, in-situ, airborne…),
- Processing centres for generating required basic products.

The main PDGS interfaces are:

- the satellite to retrieve payload data,
- the FOS to send observation plans,
- service segment to distribute low-level data and basic products and receive some auxiliary data,
- Final users to distribute low-level data and basic products mostly on manual request,
- ICS to distribute data and products for validation and calibration purpose,
- Service segment are able to interact with the PDGS observation planning system,
- CKS to receive cipher keys needed for decryption.

The main objective of the PDGS is to provide data to other entities. The PDGS shall support two different mechanisms for data distribution:

- server based, a web server authorising users to make request and download an extract of their specific needs. Other media can used in case selected product is too big for a network transfer.
- fast broadcast support, users shall receive basic products not later than 3 h from the sensing of the data.

8.6 Summary and Conclusions

The main conclusions are that the **S4/S5 ground segment is feasible** and no show-stops have been identified**.**

Nevertheless, **specific care has to be paid** to:

- the Payload Data Ground Segment (PDGS) and **the development of operational autonomous modelling and processing capabilities** allowing automatic procedures,
- **the availability of Svalbard receiving ground station** required for NRT products delivery and possibly overcrowded by the GMES space missions, the number of acquisition stations in Svalbard remains to be defined.

The main drivers for the operational atmospheric chemistry ground segment leading to these conclusions are:

- The Near Real Time (NRT) distribution of Air Quality products in 3 h to Final Users,
- The high availability required inducing the need of nearly full redundancy of the PDGS,
- The processing facilities (models…) operational status (robustness and reliability).

The data tree shall be clearly defined from raw data to the basic products to be delivered in NRT and also to the customised services requiring more complex models.

In future studies more detailed and quantified analyses will be needed on the definition of basic products and required processing facilities, as well as on the operational status of the existing models. The different level of processing shall be clearly identified and distinguished.

9 Overall Conclusions and Recommendations

In this study, CAPACITY, requirements for future atmospheric chemistry monitoring missions have been defined. The study findings support an integrated and international approach to operational monitoring of atmospheric composition to which space missions, ground-based and in-situ observations and modelling information all contribute. This overall concept is inline with the IGACO recommendations.

The complete chain from user requirements via geophysical data requirements to instrument, mission and ground segment requirements has been identified, starting from the foundation provided by the operational observing system planned for 2010-2020 (satellite and ground network) in Europe and internationally.

Candidate operational missions were evaluated taking into account the following criteria:

- The user need for operational services and urgency of the envisioned applications
- The added value over existing and planned operational systems and space elements
- The maturity of the mission concept for operational implementation

Three specific requirements for satellite observations that cannot be met by the planned operational systems have been highlighted and these include specifically a sufficient spatio-temporal sampling for the Air Quality applications, high vertical resolution measurements in the upper troposphere and lower stratosphere for the Stratospheric Ozone/Surface UV and Climate near-real time and assessment applications and measurements of climate gases (CH_4, CO, CO_2) and aerosols with sensitivity into the planetary boundary layer for Climate Protocol Monitoring.

Below we summarise the study findings per theme and give some recommendations for implementation.

Air Quality

The combination of requirements on revisit time, resolution and coverage, including frequent cloud-free sampling of the planetary boundary layer, is very stringent. The Air Quality requirements to meet user needs are not adequately addressed by the planned operational missions. Planned operational missions in LEO will contribute to, but by and large do not fulfil stringent Air Quality sampling requirements. Nominal mission lifetimes of the Envisat and EOS-Aura missions both end before 2010. Continuation of Air Quality user services based on these missions requires quick action to be taken. Moreover, planned operational missions have primarily meteorological and climate objectives. The Air Quality applications could benefit most from denser spatio-temporal sampling over Europe for forecasting and monitoring as well as globally for worldwide Air Quality monitoring and attribution of pollution episodes. The Air Quality user requirements include a suite of trace gases as well as aerosols.

CAPACITY concludes on the Air Quality theme:

- that the monitoring for operational Air Quality applications needs to be optimised with respect to the density of spatio-temporal sampling of the planetary boundary layer,
- that small ground pixels are needed to maximize (cloud-free) sampling of the boundary layer,
- that it is important to cover diurnal variations for Air Quality
- that regional coverage with short revisit time is needed to optimally serve regional Air Quality forecasting and monitoring in Europe and that global coverage is required for the monitoring and assessment of Air Quality, the oxidising capacity, and the quantification of continental in/outflow.
- that *afternoon* observations would complement best the observation times of day of MetOp and NPOESS observations in the post-Envisat/post-EOS-Aura time period

For **implementation** of the Air Quality Mission CAPACITY recommends:

- to enhance observational capabilities in the 2010-2020 time period and afterwards for operational Air Quality applications with respect to the density of spatio-temporal sampling of the planetary boundary layer by a combination of space elements in Geostationary Orbit (GEO) and Low-Earth Orbit (LEO). The global (LEO) and regional (GEO) missions are of equal importance.
    - A LEO mission with a UV-VIS-NIR-SWIR nadir viewing spectrometer with ground pixel size significantly smaller than GOME-2 and OMPS and daily global coverage in a polar orbit with *afternoon* equator crossing time optimally chosen to complement on the times of day of MetOp and NPOESS observations in the post-Envisat/post-EOS-Aura time period and to maximize (cloud-free) sampling of the boundary layer. Global coverage is required for the monitoring and assessment of Air Quality, the oxidising capacity, and the quantification of continental in/outflow.
    - A combined GEO mission with a UV-VIS-NIR-SWIR spectrometer and TIR sounder with small ground pixel sizes to cover diurnal variations in O_3, CO, NO_2, SO_2, HCHO, HNO_3, PAN, N_2O_5, organic nitrates and aerosols, height-resolved tropospheric O_3 and CO, and to significantly improve upon the cloud-free sampling of the planetary boundary layer over Europe.
    - Taking into account maturity, cost and risk issues, it is recognised that a LEO mission could have a somewhat shorter lead time, even though it will only partially fulfil the requirements of European Air Quality users.
- to prepare for phase A studies in 2005/2006 for LEO and GEO missions targeting Air Quality (Protocol Monitoring, Forecasting and Assessment) based on the given definitions of the instrument / mission concepts and requirements and their subsequent evaluation, and taking into account the importance of cloud statistics on lower tropospheric observations.

Climate Protocol Monitoring

For the monitoring of greenhouse gas and precursor emissions the planned operational missions fall short in their capabilities to observe CH_4, CO and CO_2 with sensitivity to, and frequent cloud-free sampling of the planetary boundary layer which is required to derive surface emissions. In addition, improved aerosol observations are required.

CAPACITY concludes on the Climate Protocol Monitoring theme:

- that concentration and emission monitoring is needed for O_3, NO_2, SO_2, CO_2, CO, CH_4, and aerosols
- monitoring for operational Climate Protocol applications needs to be optimised with respect to the density of spatio-temporal sampling of the planetary boundary layer,
- that small ground pixels are needed to maximize (cloud-free) sampling of the boundary layer,
- that it is limited important to cover diurnal variations for Climate protocol monitoring
- that global coverage is required, while regional coverage with short revisit time will optimally serve climate protocol monitoring in Europe.

For **implementation** of the Climate Protocol Monitoring Mission CAPACITY recommends:

- that the Air Quality Monitoring Missions (LEO and GEO) be most efficiently extended to include Climate Protocol Monitoring by addition of SWIR channels.
- to extend the phase A studies in 2005/2006 to investigate the added value of the Air Quality missions for Climate Protocol Monitoring based on the given definitions of instrument / mission concepts and requirements and their subsequent evaluation.
- that given the very stringent uncertainty requirements on CO_2 the implementation of operational monitoring of CO_2 for emission monitoring is not recommended until useful capability has been shown by the planned OCO (NASA) and GOSAT (JAXA) research missions.

Climate Monitoring, Climate Assessment and Stratospheric Ozone/Surface UV radiation
Planned operational missions fall short in the monitoring and assessment of composition-climate interactions. Specifically, it is needed to better resolve (long-term changes in) the vertical structure of the atmosphere, especially with respect to ozone and water vapour, which are very important, radiatively (climate forcing), chemically (ozone recovery, oxidizing capacity) and dynamically (Stratosphere-Troposphere connections, Brewer-Dobson circulation).
For stratospheric Ozone/Surface UV radiation planned operational missions fall short in their capability to resolve (long-term changes in) the vertical structure of the atmosphere for several long-lived compounds. Adequate vertical resolution of the order of a few kilometres in the upper troposphere and stratosphere is needed for scientific assessments of the ozone shield and would also allow improvement of the forecasting applications.

CAPACITY concludes on the Climate and Stratospheric Ozone/Surface UV radiation near-real time and assessment applications:

- that planned operational missions contribute significantly to the Protocol Monitoring ('Montreal') and near-real time ozone and UV applications
- that user needs for height-resolved data on O_3, H_2O, and other trace gases and aerosols in the upper troposphere and lower stratosphere can not be met because planned operational missions have only nadir-viewing instruments – with the exception of OMPS, which mainly targets O_3.

For **implementation** of the Climate and Stratospheric Ozone/UV radiation Near-real time and Assessment Applications CAPACITY recommends:

- to move incrementally towards an optimal operational monitoring system for these applications, in line with the GMES overall concept.
- to enhance the observational capabilities in vertical resolution in the 2010-2020 time period for the Climate and Stratospheric Ozone and Surface UV radiation near-real time and assessment applications.
- instrument specifications for limb-MIR and limb-MM techniques – feasible options with complementary capabilities – be consolidated to meet user requirements for a future operational limb-sounding component.
- to prepare for a phase A study in 2005/2006 for a limb sounding component to the LEO mission targeting Climate (Near-Real Time Monitoring and Assessment) and Stratospheric Ozone (Forecasting and Assessment) based on the conclusions drawn in the "Definition of LEO instrument / mission concepts and requirements" and its subsequent evaluation.

Alternative constellations and type of orbits
Finally, for alternative constellations and type of orbits the following general recommendation is made:

- to investigate the possibility, advantages and disadvantages of a constellation of satellites in low inclination orbit to addresses the CAPACITY operational applications in the post-EPS time frame.

Appendix: Geophysical Data Requirement Tables

Data Requirement Tables for satellite components of the specified applications A1-A3, B1-B3, C1-C3, and, for Stratospheric Ozone and Surface UV monitoring also requirement table on ‘Ground-based Observations’ (A1G).

For the full set of tables we refer to the Full Technical Note on the Derivation of Geophysical Data Requirements.

The tables as presented in the Appendix are explained in detail in Chapter 2.

A1-S

Theme: Ozone Layer
Category: Protocol Monitoring
Type of Observations: Satellite

Data Product \ Requirement	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Trend	Total column	50 / 100	--	24 / 24*3	3%
Spectral UV surface albedo	Surface UV Trend	Surface	10 / 50	--	24 / 24*3	0.1
Spectral UV solar irradiance	Surface UV Trend	Top of Atmosphere	--	--	Daily / Monthly	2%
UV Aerosol Optical Depth	Surface UV Trend	Total column	10 / 50	--	24 / 24*3	0.1
UV Aerosol Absorption Optical Depth	Surface UV Trend	Total column	10 / 50	--	24 / 24*3	0.02

A1-G

Theme: Ozone Layer
Category: Protocol Monitoring
Type of Observations: Ground-based / In-situ

Data Product \ Requirement	Driver	Height Range	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Validation	Total column	--	24 / 24*3	3%
UV Index	Validation	Surface	--	Daily maximum	0.5 (UVI <=5) 10% (UVI > 5)
UV dose	Validation	Surface	--	Daily dose	0.5 $kJ.m^{-2}$
CFC-11	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	2% (ZA) 2% (ZA)
CFC-12	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	2% (ZA) 2% (ZA)
CFC-113	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	2% (ZA) 2% (ZA)
HCFC-22	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	5% (ZA) 5% (ZA)
HCFC-141b	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	5% (ZA) 5% (ZA)
HCFC-142b	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	5% (ZA) 5% (ZA)
CCl_4	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	2% (ZA) 2% (ZA)
CH_3CCl_3	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	2% (ZA) 2% (ZA)
Halon 1211	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	2% (ZA) 2% (ZA)
Halon 1301	Trend	Surface Total column	PBL --	24 / 24*7 24 / 24*7	2% (ZA) 2% (ZA)

A2-S

Theme: Ozone Layer
Category: Near-Real Time Data
Type of Observations: Satellite

Data Product \ Requirement	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Ozone and UV Forecast	UT	20 / 100	0.5 / 2	6 / 24*3	20%
		LS	50 / 100	0.5 / 2	6 / 24*3	20%
		MS	100 / 200	2 / 3	6 / 24*3	20%
		US+M	100 / 200	3 / 5	12 / 24*7	20%
		Troph. column	10 / 50	--	6 / 24*3	20%
		Total column	50 / 100	--	6 / 24*3	5%
Spectral UV surface albedo	UV Forecast	Surface	10 / 50	--	6 / 24*3	0.1
Spectral UV solar irradiance	UV Forecast	Top of Atmosphere	--	--	Daily / Monthly	2%
UV Aerosol Optical Depth	UV Forecast	Total column	10 / 50	--	6 / 24*3	0.1
UV Aerosol Absorption Optical Depth	UV Forecast	Total column	10 / 50	--	6 / 24*3	0.02
Strat. Aerosol Optical Depth	Ozone loss	LS	50 / 100	0.5 / 2	6 / 24*3	0.05
		MS	50 / 200	1 / 3	12 / 24*7	0.05
		Stratosphere	50 / 200	--	6 / 24*7	0.05
ClO	Ozone loss	LS	50 / 200	2 / part. column	24 / 24*7	50%
		MS	100 / 200	2 / part. column	24 / 24*7	50%
		Stratosphere	50 / 200	--	24 / 24*7	50%
NO_2	Ozone loss	LS	50 / 200	2 / part. column	24 / 24*7	20%
		MS	100 / 200	2 / part. column	24 / 24*7	20%
		Stratosphere	50 / 200	--	24 / 24*7	20%
PSC occurrence	Ozone loss	LS	50 / 100	0.5 / 2	6 / 24*3	< 10% mis-assignments
SF_6	Tracer	LS	50 / 200	1 / 2	6 / 24*3	10%
		MS	100 / 200	2 / 3	12 / 24*7	10%
CO_2 (as tracer alternative to SF6)	Tracer; Radiation budget	LS	50 / 200	1 / 2	6 / 24*3	10%
		MS	100 / 200	2 / 3	12 / 24*7	10%
H_2O	Radiation budget; ST exchange	UT	20 / 100	0.5 / 2	6 / 24*3	20%
		LS	50 / 100	1 / 2	6 / 24*3	20%
		MS	100 / 200	2 / 3	12 / 24*7	20%
N_2O (as tracer alternative to SF6)	Tracer; Radiation budget	LS	50 / 100	1 / 2	6 / 24*3	20%
		MS	50 / 200	2 / 3	12 / 24*7	20%
		US	50 / 200	3 / 5	12 / 24*7	20%
CH_4 (as tracer alternative to SF6)	Tracer; Radiation budget	LS	50 / 200	1 / 2	6 / 24*3	20%
		MS	100 / 200	2 / 3	12 / 24*7	20%
HCl	ST exchange	LS	Co-located with O3	Co-located with O3	Co-located with O3	20%
HNO_3	ST exchange	LS	Co-located with O3	Co-located with O3	Co-located with O3	20%
CO	ST exchange	UT+LS	Co-located with O3	Co-located with O3	Co-located with O3	20%

A3-S	Theme: Category: Type of Observations:				Ozone Layer Assessment Satellite	
Requirement / Data Product	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Ozone and UV Trend; Ozone loss; Surface UV, Ozone-Climate interaction	UT LS MS US+M Troph. column Total column	20 / 100 50 / 100 100 / 200 100 / 200 10 / 50 50 / 100	1 / 3 1 / 3 2 / 3 3 / 5 -- --	6 / 24*3 6 / 24*3 6 / 24*3 6 / 24*7 6 / 24*3 6 / 24*3	20% 10% 20% 20% 20% 10%
Spectral UV surface albedo	Surface UV	Surface	10 / 50	--	6 / 24*3	0.1
UV Aerosol Optical Depth	Surface UV	Total column	10 / 50	--	6 / 24*3	0.1
UV Aerosol Absorpton Optical Depth	Surface UV	Total column	10 / 50	--	6 / 24*3	0.02
Spectral UV solar irradiance	Surface UV	Top of Atmosphere	--	--	monthly	2%
H_2O	Ozone-Climate interaction	LS MS US Stratosphere	50 / 100 100 / 200 100 / 200 50 / 200	1 / 3 2 / 3 3 / 5 --	12 / 24*3 12 / 24*7 12 / 24*7 12 / 24*7	15% (1000 km) 15% (1000 km) 15% (1000 km) 15% (1000 km)
N_2O	Ozone-Climate interaction	LS MS US Stratosphere	50 / 100 100 / 200 100 / 200 50 / 200	1 / 3 2 / 3 3 / 5 --	12 / 24*3 12 / 24*7 12 / 24*7 12 / 24*7	10% (ZA) 10% (ZA) 10% (ZA) 10% (ZA)
CH_4	Ozone-Climate interaction	LS MS US Stratosphere	50 / 100 100 / 200 100 / 200 50 / 200	1 / 3 2 / 3 3 / 5 --	12 / 24*3 12 / 24*7 12 / 24*7 12 / 24*7	10% (ZA) 10% (ZA) 10% (ZA) 10% (ZA)
HNO_3	Ozone Trend; Dinitrification	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	30% (1000 km) 30% (1000 km) 30% (1000 km)
CFC-11	Ozone trend	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	5% (ZA) 5% (ZA) 5% (ZA)
CFC-12	Ozone trend	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	5% (ZA) 5% (ZA) 5% (ZA)
HCFC-22	Ozone trend	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	20% (ZA) 20% (ZA) 20% (ZA)
ClO	Ozone loss	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	30% (1000 km) 30% (1000 km) 30% (1000 km)
BrO	Ozone loss	LS MS Stratosphere	50 / 100 100 / 200 50 / 200	1 / 3 2 / 3 --	12 / 24*3 12 / 24*7 12 / 24*7	30% (1000 km) 30% (1000 km) 30% (1000 km)
NO_2	Ozone loss	LS MS	50 / 100 100 / 200	1 / 3 2 / 3	12 / 24*3 12 / 24*7	30% (1000 km) 30% (1000 km)

		Stratosphere	50 / 200	--	12 / 24*7	30% (1000 km)
Aerosol surface density	Ozone loss	LS	50 / 100	1 / 3	12 / 24*3	100% (1000 km)
		MS	100 / 200	2 / 3	12 / 24*7	100% (1000 km)
		Stratosphere	50 / 200	--	12 / 24*7	100% (1000 km)
PSC occurrence	Ozone loss	LS	50 / 100	1 / 3	12 / 24*3	< 10% mis-assignments
HCl	Chlorine trend	LS	50 / 100	1 / 3	12 / 24*3	30% (1000 km)
		MS	100 / 200	2 / 3	12 / 24*7	30% (1000 km)
		Stratosphere	50 / 200	--	12 / 24*7	30% (1000 km)
$ClONO_2$	Chlorine trend	LS	50 / 100	1 / 3	12 / 24*3	30% (1000 km)
		MS	100 / 200	2 / 3	12 / 24*7	30% (1000 km)
		Stratosphere	50 / 200	--	12 / 24*7	30% (1000 km)
HBr	Bromine trend	LS	50 / 100	1 / 3	12 / 24*3	30% (1000 km)
		MS	100 / 200	2 / 3	12 / 24*7	30% (1000 km)
		Stratosphere	50 / 200	--	12 / 24*7	30% (1000 km)
$BrONO_2$	Bromine trend	LS	50 / 100	1 / 3	12 / 24*3	30%
		MS	100 / 200	2 / 3	12 / 24*7	30%
		Stratosphere	50 / 200	--	12 / 24*7	30%
CH_3Cl	Bromine trend	LS	50 / 100	1 / 3	12 / 24*3	30%
		MS	100 / 200	2 / 3	12 / 24*7	30%
		Stratosphere	50 / 200	--	12 / 24*7	30%
CH_3Br	Bromine trend	LS	50 / 100	1 / 3	12 / 24*3	5% (ZA)
		MS	100 / 200	2 / 3	12 / 24*7	5% (ZA)
		Stratosphere	50 / 200	--	12 / 24*7	5% (ZA)
SO_2 enhanced	Ozone loss	LS	50 / 100	1 / 3	12 / 24*3	50%
		MS	100 / 200	2 / 3	12 / 24*7	50%
		Stratosphere	50 / 200	--	12 / 24*7	50%
Volcanic aerosol	Ozone loss	LS	50 / 100	1 / 3	12 / 24*3	
		MS	100 / 200	2 / 3	12 / 24*7	< 10% mis-assignments
		Stratosphere	50 / 200	--	12 / 24*7	

B1-S

Theme: **Air Quality**
Category: **Protocol Monitoring**
Type of Observations: **Satellite**

Data Product \ Requirement	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Interpolation of Surface network; Boundary condition; UV actinic fluxes	PBL	5 / 20	--	0.5 / 2	10%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	25%
		Total Column	50 / 100	--	24 / 24*3	3%
NO_2	Interpolation of Surface network; Emissions; Boundary condition	PBL	5 / 20	--	0.5 / 2	10%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
CO	Interpolation of Surface network; Emissions; Boundary condition	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	25%
		Total Column	5 / 20	--	0.5 / 2	25%
SO_2	Interpolation of Surface network; Emissions; Boundary condition	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
CH_2O	Interpolation of Surface network; VOC Emissions; Boundary condition	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
Aerosol OD	Interpolation of Surface network; Emissions; Boundary condition; UV actinic fluxes	PBL	5 / 20	--	0.5 / 2	0.05
		FT	5 / 50	--	0.5 / 2	0.05
		Tropospheric Column	5 / 20	--	0.5 / 2	0.05
		Total Column	5 / 20	--	0.5 / 2	0.05
Aerosol Type	Translation Aerosol OD to PM surface concentrations	PBL	5 / 20	--	0.5 / 2	< 10% mis-assignments
		FT	5 / 50	--	0.5 / 2	< 10% mis-assignments
		Tropospheric Column	5 / 20	--	0.5 / 2	< 10% mis-assignments
		Total Column	5 / 20	--	0.5 / 2	< 10% mis-assignments

B2-S

Theme:	Air Quality
Category:	Near-Real Time Data
Type of Observations:	Satellite

Requirement / Data Product	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Air Quality Forecast; UV actinic fluxes	PBL	5 / 20	--	0.5 / 2	10%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	25%
		Total Column	50 / 100	--	12 / 24*3	5%
NO_2	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	10%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
CO	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Ttropospheric Column	5 / 20	--	0.5 / 2	25%
		Total Column	5 / 20	--	0.5 / 2	25%
Aerosol OD	Air Quality Forecast; UV actinic fluxes	PBL	5 / 20	--	0.5 / 2	0.05
		FT	5 / 50	--	0.5 / 2	0.05
		Ttropospheric Column	5 / 20	--	0.5 / 2	0.05
		Total Column	5 / 20	--	0.5 / 2	0.05
Aerosol Type	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	< 10% mis-assignments
		FT	5 / 50	--	0.5 / 2	< 10% mis-assignments
		Ttropospheric Column	5 / 20	--	0.5 / 2	< 10% mis-assignments
		Total Column	5 / 20	--	0.5 / 2	< 10% mis-assignments
H_2O	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	10%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	10%
		Total Column	5 / 20	--	0.5 / 2	10%
SO_2	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
CH_2O	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
HNO_3	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
N_2O_5 (night)	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	50%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
PAN	Air Quality Forecast	PBL	5 / 20	--	0.5 / 2	20%
		FT	5 / 50	1 / 3	0.5 / 2	20%
		Tropospheric Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2

		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
Spectral UV surface albedo	UV actinic fluxes	Surface	5 / 20	--	24 / 24*3	0.1

B3-S

Theme: Air Quality
Category: Assessment
Type of Observations: Satellite

Data Product \ Requirement	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Phot. Acitivity; Ox. Capacity; Background	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	10% 20% 25% 3%
NO_2	Emissions; Phot. Acitivity; Ox. Capacity	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	10% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2
CO (+ isotopes)	Ox. Capacity; Emissions; Background	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 25% 25%
Aerosol OD	Emissions; UV actinic fluxes	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- -- -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	0.05 0.05 0.05 0.05
Aerosol Type	Emissions	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- -- -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	< 10% mis-assignments < 10% misassignments < 10% mis-assignments < 10% mis-assignments
H_2O	Ox. Capacity	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	10% 20% 10% 10%
SO_2	Emissions	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2
CH_2O	Phot. Activity; VOC emissions	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2
HNO_3	Ox. Capacity	PBL FT Tropospheric Column	5 / 20 5 / 50 5 / 20	-- 1 / 3 --	0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2

		Total Column	5 / 20	--	0.5 / 2	1.3e15 molec cm-2
N_2O_5 (nighttime)	Ox. Capacity	PBL FT Tropospheric Column Total Column	5 / 20 5 / 50 5 / 20 5 / 20	-- 1 / 3 -- --	0.5 / 2 0.5 / 2 0.5 / 2 0.5 / 2	20% 20% 1.3e15 molec cm-2 1.3e15 molec cm-2
Organic Nitrates	Ox. Capacity	PBL	5 / 20	--	0.5 / 2	30%
Spectral UV surface albedo	UV actinic fluxes	Surface	5 / 20	--	24 / 24*3	0.1

C1-S

Theme: **Climate**
Category: **Protocol Monitoring**
Type of Observations: **Satellite**

Requirement / Data Product	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
CO_2 (PBL sensitive)	Emissions	Tropospheric column Total column	10 / 50 10 / 50	-- --	6 / 12 6 / 12	0.5% 0.5%
CH_4 (PBL sensitive)	Emissions	Tropospheric column Total column	10 / 50 10 / 50	-- --	24 / 24*3 24 / 24*3	2% 2%
O_3	Radiative forcing	Troposphere Tropospheric column Total column	10 / 50 10 / 50 50 / 100	2 / 5 -- --	12 / 24*3 12 / 24*3 24 / 24*3	20% 25% 3%
NO_2 (PBL sensitive)	Emissions	Troposphere Tropospheric column Total column	10 / 50 10 / 50 10 / 50	2 / 5 -- --	12 / 24*3 12 / 24*3 12 / 24*3	50% 1.3·(10)15 cm^{-} 1.3·(10)15 cm^{-2}
CO (PBL sensitive)	Emissions	Troposphere Tropospheric column Total column	10 / 50 10 / 50 10 / 50	2 / 5 -- --	12 / 24*3 12 / 24*3 12 / 24*3	20% 25% 25%
Aerosol OD	Emissions; Radiative forcing	Troposphere LS MS Total column	10 / 50 50 / 100 50 / 200 10 / 50	-- 1 / part. column 2 / part. column --	6 / 24*3 12 / 24*3 12 / 24*3 12 / 24*3	0.05 0.05 0.05 0.05
Aerosol absorption OD	Radiative forcing	Troposphere Total column	10 / 50 10 / 50	-- --	6 / 24*3 6 / 24*3	0.01 0.01

C2-S

Theme:	**Climate**
Category:	**Near-Real Time Data**
Type of Observations:	**Satellite**

Data Product \ Requirement	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Radiation; Dynamics	PBL	5 / 50	--	6 / 24	30%
		Tropospheric column	10 / 50	--	6 / 24*3	25%
		LS	50 / 100	0.5 / 2	6 / 24*3	10%
		MS	50 / 200	1 / 3	6 / 24*7	20%
		US+M	50 / 200	3 / 5	6 / 24*7	20%
		Total column	50 / 100	--	6 / 24*3	5%
H_2O	Radiation; Dynamics; Hydrological cycle; Stratospheric H2O	PBL	5 / 50	--	1 / 6	50%
		FT	10 / 50	0.5 / 2	1 / 6	30%
		UT	10 / 100	0.5 / 2	1 / 6	30%
		LS	50 / 100	0.5 /2	3 / 24	20%
		MS	50 / 200	1 / 3	6 / 24*7	20%
		US	50 / 200	3 / 5	6 / 24*7	20%
		Total column	10 / 50	--	6 / 24*3	5%
CO_2	Radiation; Tracer	PBL	5 / 50	--	6 / 12	10%
		MS	50 / 200	1 / 3	12 / 24*7	10%
		US	50 / 200	1 / 3	12 / 24*7	10%
		Total column	1 / 20	--	1 / 12	2%
CH_4	Radiation; Tracer	LS	50 / 100	1 / 3	12 / 24*3	20%
		MS	50 / 200	1 / 3	12 / 24*3	20%
		Total column	10 / 50	--	12 / 24*3	2%
N_2O	Radiation; Tracer	LS	50 / 100	1 / 3	12 / 24*3	20%
		MS	50 / 200	1 / 3	12 / 24*3	20%
		US	50 / 200	3 / 5	12 / 24*3	20%
		Total Column	10 / 50	--	12 / 24*3	2%
Aerosol OD	Radiation	PBL	5 / 10	--	1 / 6	0.05
		Troposphere	5 / 50	--	3 / 24	0.05
		LS	50 / 100	1 / part. column	12 / 24*3	0.05
		MS	50 / 200	1 / part. column	12 / 24*3	0.05
Aerosol absorption OD	Radiation	PBL	5 / 10	--	1 / 6	0.01
		Troposphere	5 / 50	--	3 / 24	0.01
Cirrus OD	Radiation	UT	10 / 100	--	6 / 24	100%
SF_6	Tracer	LS	50 / 100	1 / 3	12 / 24*7	10%
		MS	50 / 200	1 / 3	12 / 24*7	10%
		US	50 / 200	3 / 5	12 / 24*7	10%
HDO	Tracer; Stratospheric H2O	LS	50 / 100	1 / 3	12 / 24*7	10%
		MS	50 / 200	1 / 3	12 / 24*7	10%
		US	50 / 200	3 / 5	12 / 24*7	10%
HF (alternative tracer)	Tracer	LS	50 / 100	1 / 3	12 / 24*7	10%
		MS	50 / 200	1 / 3	12 / 24*7	10%
		US	50 / 200	3 / 5	12 / 24*7	10%
Aerosol phase function	Radiation	PBL	5 / 10	--	1 / 6	0.1 on asymmetry factor
		Troposphere	5 / 50	--	3 / 24	0.1 on asymmetry factor

Cirrus phase function	Radiation	UT	10 / 100	--	6 / 24	0.1 on asymmetry factor

C3-S

Theme:	**Climate**
Category:	**Assessment**
Type of Observations:	**Satellite**

Data Product \ Requirement	Driver	Height Range	Horizontal resolution (km)	Vertical resolution (km)	Revisit Time (hours)	Uncertainty
O_3	Radiative Forcing; Oxidising Capacity; Tracer; Ozone recovery	Troposphere	10 / 50	1 / 3	6 / 24*3	30%
		Tropospheric Column	10 / 50	--	6 / 24*3	25%
		UT	20 / 100	0.5 / 2	6 / 24*3	20%
		LS	50 / 100	0.5 / 2	6 / 24*3	20%
		MS	50 / 100	2 / 3	6 / 24*3	20%
		US+M	100 / 200	3 / 5	6 / 24*7	20%
		Total Column	50 / 100	--	6 / 24*3	3%
H_2O	Radiative Forcing; Oxidising Capacity; Tracer; O3 recovery; Stratospheric H2O	PBL	1 / 20	--	6 / 24	30%
		Troposphere	10 / 50	1 / 3	6 / 24*3	30%
		Tropospheric Column	10 / 50	--	6 / 24*3	10%
		UT	20 / 100	0.5 / 2	6 / 24*3	20%
		LS	50 / 100	0.5 / 2	6 / 24*3	20%
		MS	50 / 100	2 / 3	6 / 24*7	20%
		US+M	100 / 200	3 / 5	6 / 24*7	20%
		Total Column	50 / 100	--	6 / 24*3	10%
CO_2	Radiative Forcing; Tracer	MS	50 / 100	2 / 3	12 / 24*3	10%
		Total Column (PBL sensitive)	10 / 50	--	1 / 12	0.5%
CH_4	Radiative Forcing; Oxidising Capacity; Tracer; Stratospheric H2O	LS	50 / 100	1 / 3	12 / 24*3	20%
		MS	50 / 100	2 / 3	12 / 24*3	20%
		Total Column (PBL sensitive)	10 / 50	--	12 / 24*3	2%
N_2O	Radiative Forcing; Tracer; N budget	LS	50 / 100	1 / 3	12 / 24*3	20%
		MS	50 / 100	2 / 3	12 / 24*3	20%
		US	50 / 100	3 / 5	12 / 24*7	20%
		Total Column (PBL sensitive)	10 / 50	--	12 / 24*3	2%
CO	Ozone and CO2 precursor	Troposphere	10 / 50	1 / 3	12 / 24*3	30%
		Troposph. Col. (PBL sensitive)	10 / 50	--	12 / 24*3	25%
		UT	20 / 100	1 / 3	12 / 24*3	20%
		LS	50 / 100	1 / 3	12 / 24*3	20%
NO_2	Ozone and Aerosol precursor	Troposphere	10 / 50	1 / 3	6 / 24*3	30%
		Troposph. Col. (PBL sensitive)	10 / 50	--	12 / 24*3	1.3·(10)15 cm^{-2}
		UT	20 / 100	1 / 3	6 / 24*3	50%
		LS	50 / 100	1 / 3	12 / 24*3	50%
		MS	50 / 200	2 / 3	12 / 24*3	30%
		Total Column	50 / 100	--	12 / 24*3	10%
CH_2O	Oxidising Capacity	Troposphere	10 / 50	1 / 3	6 / 24*3	30%
		Troposph. Col. (PBL sensitive)	10 / 50	--	12 / 24*3	1.3·(10)15 cm^{-2}
		UT	20 / 100	1 / 3	6 / 24*3	30%
		Total Column (PBL sensitive)	10 / 50	--	12 / 24*3	1.3·(10)15 cm^{-2}
HNO_3	N budget	Troposphere	10 / 50	1 / 3	6 / 24*3	30%
		UT	20 / 100	1 / 3	6 / 24*3	20%
		LS	50 / 100	1 / 3	12 / 24*3	20%
		MS	50 / 200	2 / 3	12 / 24*3	20%
		Total Column	10 / 50	--	12 / 24*3	20%

Cirrus OD	Radiative Forcing	UT	10 / 100	--	6 / 24	100%
PSC occurrence (day + night)	Radiative Forcing	LS	50 / 100	0.5 / 2	6 / 24*3	< 10% mis-assignments
Aerosol OD	Radiative Forcing	PBL Troposphere LS MS Total Column	5 / 20 10 / 50 50 / 100 50 / 200 10 / 50	-- -- 1 / part. column 2 / part. column --	6 / 24 6 / 24 12 / 24*3 12 / 24*3 12 / 24*3	0.05 0.05 0.05 0.05 0.05
Aerosol absorption OD	Radiative Forcing	Troposphere Total Column	5 / 50 5 / 50	-- --	6 / 24 6 / 24	0.01 0.01
Spectral solar irradiance	Radiative Forcing	Top of Atmosphere	--	--	24 / 24*7	2%
HCl	Ozone recovery	LS	50 / 100	1 / 3	12 / 24*3	20%
CH_3Cl	Ozone recovery	LS MS Stratosphere	50 / 100 50 / 200 50 / 100	1 / 3 2 / 3 --	12 / 24*3 12 / 24*3 12 / 24*3	20% 20% 20%
CH_3Br	Ozone recovery	LS MS Stratosphere	50 / 100 50 / 200 50 / 100	1 / 3 2 / 3 --	12 / 24*3 12 / 24*3 12 / 24*3	20% 20% 20%
SF_6	Tracer	LS MS US	50 / 100 50 / 200 50 / 200	1 / 3 2 / 3 3 / 5	12 / 24*7 12 / 24*7 12 / 24*7	10% 10% 10%
HDO	Tracer; Stratospheric H2O	LS MS US Stratosphere	50 / 100 50 / 200 50 / 200 50 / 100	1 / 3 2 / 3 3 / 5 --	12 / 24*7 12 / 24*7 12 / 24*7 12 / 24*7	10% 10% 10% 10%
HF	Tracer	LS MS US	50 / 100 50 / 200 50 / 200	1 / 3 2 / 3 3 / 5	12 / 24*7 12 / 24*7 12 / 24*7	10% 10% 10%
CFC-11	Radiative Forcing	LS MS Stratosphere	50 / 100 50 / 200 50 / 100	1 / 3 2 / 3 --	12 / 24*7 12 / 24*7 12 / 24*7	20% 20% 20%
CFC-12	Radiative Forcing	LS MS Stratosphere	50 / 100 50 / 200 50 / 100	1 / 3 2 / 3 --	12 / 24*7 12 / 24*7 12 / 24*7	20% 20% 20%
HCFC-22	Radiative Forcing	UT LS MS Stratosphere	20 / 100 50 / 100 50 / 200 50 / 100	1 / 3 1 / 3 2 / 3 --	12 / 24*3 12 / 24*3 12 / 24*3 12 / 24*3	20% 20% 20% 20%
H_2O_2	Oxidising Capacity	Troposphere UT	10 / 50 20 / 100	1 / 3 1 / 3	6 / 24*3 6 / 24*3	30% 30%
N_2O_5	N budget	Troposphere UT LS MS Stratosphere	10 / 50 20 / 100 50 / 100 50 / 200 50 / 100	-- 1 / 3 1 / 3 1 / 3 --	6 / 24*3 6 / 24*3 12 / 24*3 12 / 24*3 12 / 24*3	30% 30% 50% 50% 50%
PAN	N budget	Troposphere UT Total column	10 / 50 20 / 100 10 / 50	-- 1 / 3 --	6 / 24*3 6 / 24*3 6 / 24*3	30% 30% 30%
CH_3COCH_3	Oxidising Capacity	Troposphere UT Total column	10 / 50 20 / 100 10 / 50	-- 1 / 3 --	6 / 24*3 6 / 24*3 6 / 24*3	30% 30% 30%
C_2H_6	Oxidising Capacity	Troposphere UT Total column	10 / 50 20 / 100 10 / 50	-- 1 / 3 --	6 / 24*3 6 / 24*3 6 / 24*3	50% 50% 50%
ClO (for enhanced levels)	Ozone Recovery	LS MS Stratosphere	50 / 100 50 / 200 50 / 100	1 / 3 2 / 3 --	12 / 24*3 12 / 24*3 12 / 24*3	20% 20% 20%
ClONO2	Ozone Recovery	LS	50 / 100	1 / 3	12 / 24*3	20%

		MS	50 / 200	2 / 3	12 / 24*3	20%
		Stratosphere	50 / 100	--	12 / 24*3	20%
SO_2 (for enhanced levels)	Volcanoes	Troposphere	10 / 50	1 / 3	6 / 24*3	50%
		LS	50 / 100	1 / 3	12 / 24*3	50%
		MS	50 / 200	2 / 3	12 / 24*3	50%
		Total column	10 / 50	--	6 / 24*3	50%
Aerosol phase function	Radiative Forcing; Volcanoes	Troposphere	10 / 50	--	6 / 24	0.1 on asymmetry factor
		LS	50 / 100	1 / part. column	12 / 24*3	0.1 on asymmetry factor
		MS	50 / 200	2 / part. column	12 / 24*3	0.1 on asymmetry factor
		Total column	10 / 50	--	6 / 24	0.1 on asymmetry factor
Cirrus phase function	Radiative Forcing	UT	10 / 100	--	6 / 24	0.1 on asymmetry factor