CAMELOT Final Report
Issue 1

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Distribution list:

Camelot Study Team

ESA
Joerg Langen (Technical Officer) ESA-ESTEC
Helene Etienne (Contracts Officer) ESA-ESTEC

External
Rosemary Munro EUMETSAT

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ESA STUDY CONTRACT REPORT

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ABSTRACT

This is the final report of the CAMELOT (Chemistry of the Atmosphere Mission concEpts and sentineL Observations Techniques) study. The key objective of the CAMELOT study was to contribute to the definition of the air quality and climate protocol monitoring parts of GMES Sentinels 4 and 5 missions. This report presents the conclusions and recommendations of this study, regarding the Sentinel 4 and 5 Level 1B requirements and the mission scenario's.

NAMES OF AUTHORS:

P.F. Levelt, J.P. Veefkind – Royal Netherlands Meteorological Institute, De Bilt, The Netherlands
B.J. Kerridge, R. Siddans, Rutherford Appleton Laboratory, Chilton, Didcot, UK
G. de Leeuw, Finnish Meteorological Institute, Helsinki, Finland
J. Remedios, University of Leicester, Leicester, UK
P.F. Coheur, Free University of Brussels, Brussels, Belgium

ESA STUDY MANAGER: J. Langen **DIVISION:** EOP-SM **DIRECTORATE:** EOP	**ESA BUDGET HEADING:**

Executive Summary

This report presents the summary of the ESA CAMELOT (Chemistry of the Atmosphere Mission concEpts and sentineL Observations Techniques). The key objective of the CAMELOT study was to contribute to the definition of the air quality and climate protocol monitoring parts of GMES Sentinels 4 and 5 in the time frame 2012-2020. In particular the MRD user requirements Tables B1, B2 and C1 were in scope of the CAMELOT study. These tables define the user requirements for air quality protocol monitoring, air-quality near-real-time applications, and climate protocol monitoring. The ozone layer user requirements (Tables A1, A2 and A3), the air quality assessment (Table B3) as well as the climate near-real-time and climate assessment (Tables C2 and C3) were out of scope for the CAMELOT study.

In CAMELOT, the following aspects have been studied

- Complementation of the geophysical observation requirements of the CAPACITY study by generation of meteorological and possibly other auxiliary data requirements and delivery time requirements;
- Contributions to trade-offs among different observation principles for several chemical species and parameters;
- Derivation of comprehensive instrument performance requirements from the geophysical observation requirements with previously identified observation principles, including in-depth study of implementation-critical requirements;
- Quantification of the effects of cloud interference as a function of geophysical and observational parameters;
- Optimisation of orbit scenarios and contributions to the trade-off between them;
- Support to parallel Sentinel 4 and 5 phase 0 and phase A system studies;
- Recommendations for changes and additions in the Mission Requirements Documents.

The CAMELOT study the following tasks have been performed:

- Task1: Preparation of geophysical scenarios for simulations;
- Task 2: Complementary observations and delivery requirements;
- Task 3: Retrieval simulations;
- Task 4: Assessment of cloud contamination;
- Task 5: Optimisation of mission scenario’s;
- Task 6: Support to Sentinel 4 and 5 Phase 0 and Phase A system studies;
- Task 7: Conclusions and recommendations.

The CAMELOT study has resulted in detailed results in support of the Sentinel 4 and 5 missions. For the assessment of the user requirements the MRD Tables B1, B2 and C1, addressing air quality protocol monitoring, near-real-time and climate protocol monitoring applications, were in scope for the study.

Within the CAMELOT study datasets of four-dimensional fields of aerosol and trace gases have been produced using state-of-the-art chemistry-transport and climate models. The spatial-temporal variability in these is larger than the variability due to the different IPCC emission scenarios. Therefore, the selected profiles, which span a wide range of trace gas and aerosol concentrations, are representative for the current as well the future variability in trace gas and aerosol concentrations.

The CAMELOT study has considered auxiliary variables, which need to be measured in order to deliver the required output product quality for the Sentinel 4/5 system. These include auxiliary information required for product development in the ground segment, for quality control/quality assurance (QA/QC) and for the application areas of air quality and climate. Considering the auxiliary data needs, the following conclusion have been reached:

- For product development cloud and aerosol determination is very important. Other new auxiliary data requirements noted were for surface albedo/emissivity maps and digital elevation models in the ground segment as well as meteorological analysis/forecast data. If vertical column densities are to be provided, e.g. for NO_2, a chemical-transport model or its outputs needs to be included in the ground segment.

- For QA/QC, validation requirements are maturing at a reasonable rate. There are, however, some critical issues, which include ensuring the accuracy and consistency of air quality measurements in the urban areas and for greenhouse gases for climate. For air quality, the key issue is a representative, long-term operational network for NO_2 with verifiable performance.
- Based on a user survey and literature, it is suggested that a satellite product estimating the photolysis rates for NO2 should be produced. For the photolysis product, aerosol and cloud optical depth are additional data sets, which are required, and these would offer extra capabilities to the air quality model.
- A survey of users in the air quality area and published air quality reports showed the prevalence of use of daily image data of the MODIS form. Other desirable aspects included requirements for aerosol with dust separation, fire maps, land cover and land surface temperature. Sentinel 3 data are recognised to be an important future source for these data sets and support should be given to production of the appropriate data sets for atmosphere applications.
- Applications in the climate area emphasized the importance of producing mean dry mole fraction or mean dry air mixing ratio for methane and carbon dioxide. The corresponding auxiliary data requirements for methane are for O_2 and CO_2 columns (surface pressure) for normalisation to mean dry air mixing ratios. For auxiliary data for greenhouse gas inverse modelling and for assimilation of greenhouse gases, the most important parameters are fire (burned area), land cover maps, vegetation intensity indication for land; ocean colour and sea surface temperature for the ocean; atmospheric chemistry observations which constrain OH. Note that CO measurements are required for CH_4 inverse modelling since CH_4 and CO are inter-linked as per the CAPACITY study findings.

The CAMELOT study has investigated the time requirements for the delivery of near-real-time data users. For NWP/UV forecast applications, an estimated 4 hours acceptable delay time for NWP purposes is sufficient. For air quality forecast and monitoring, at least a delivery time of 3 hours maximum is required. In the case of ozone and tropospheric aerosols, somewhat relaxed delivery times may be acceptable, with ozone estimated 5 hours and aerosol about 8 hours. No clear indication of preference could be gained from users for the hour of delivery. However, with sensors operating in the UV-VIS range, late afternoon delivery is a preferable choice.

In the CAMELOT, the Level 1B requirements for the foreseen instruments on the Sentinel 4 and 5 have been derived using retrieval simulations as the most important tool. On the Level 1B requirements, the CAMELOT study has reached the following conclusions and recommendations:

- It is recommended to update the MRD requirements according to the recommendations given in the CAMELOT final report and the underlying Task 3 task reports. For the UVN instruments the recommendations are mainly refinements of the initial MRD requirements. For TIR it is recommended to make a considerable update based on the study results, IASI experience and the homogenisation between Sentinel 5 and Post-EPS MRD. For the SWIR instrument on Sentinel 5 it is recommended to revise several Level 1B requirements. An important recommendation for the SWIR spectrometer is to increase the priority of the 1.6 μm band to priority 1, in order to enable three band retrievals for methane. The 1.6 μm band may also be used for the retrieval of CO_2, for which the retrieval simulations showed good performance with some limitations for cirrus and aerosol cases. The GOSAT mission should confirm these findings for the retrieval of CO_2.
- The user requirements for sulphur dioxide and formaldehyde will not be met with a realistic UVN spectrometer. Although these measurements of formaldehyde and sulphur dioxide do not meet the user requirements for individual measurements, they will be used after temporal and/or spatial averaging to improve the emission inventories, which are an essential input for air quality and chemistry-transport models.
- It is recommended to review some of the user requirements given in the MRD. The consensus of the CAMELOT consortium was that the user requirements for the total and tropospheric column of CO are too relaxed. For formaldehyde and sulphur dioxide the requirement were seen as too strict. Also, it is recommended to review the user requirements for HNO_3 and PAN. It may be considered to specify the user requirement for CO_2 in more detail. In addition, it should be considered to add user requirements

for amongst others ammonia and glyoxal, for which the feasibility of satellite based observations has been demonstrated.

- It is recommended to include in the Sentinel 5 mission the UV-TIR and SWIR-TIR spectral ranges needed for the combined retrievals of ozone and carbon monoxide, which offer theoretically significant improvements in the troposphere and the PBL. For that purpose, the spatial co-alignment between the UV and TIR, and the SWIR and the TIR ground pixels should be of the order of a few kilometres, matching the expected ozone and carbon monoxide tropospheric variability. The temporal requirements are of the order of a few minutes. Therefore, it is recommended to put the UV, SWIR and TIR spectrometers on the same satellite platform.

- It is recommended to develop the combined retrievals for real data using IASI and GOME-2 data and TES or AIRS and OMI data. The retrievals on data from these instruments should demonstrate the feasibility of the ozone combined retrievals for monitoring purposes.

- In support for the combined UV-TIR ozone retrievals and SWIR-TIR carbon monoxide retrievals, consistent spectroscopic laboratory measurements for these wavelength bands are needed at the relevant atmospheric temperatures and pressures.

- The sensitivity of UVN observations to boundary layer ozone is low. In combination with the relatively small contribution of the boundary layers ozone to the tropospheric column, polluted boundary layers can only be observed for very strong pollution events, in combination with high boundary layers. The diurnal variations in ozone are predominantly confined to the boundary layer. Therefore, the observation of the diurnal variation in ozone by the Sentinel 4 UVN will be limited to specific cases for large Mediterranean cities during pollution events, for which high ozone concentrations and thick boundary layers can occur.

- To measure the aerosol optical thickness up to the user requirements and to derive aerosol type information, a directional polarization instrument should be added to the Sentinel 5. The UVN instrument alone cannot make the aerosol observations that meet the user requirements. Such an instrument has strong synergy with the NIR channel of the UVN instrument, because of the aerosol height information in the O_2-A band. This synergy can be exploited if the directional polarization instrument and the UVN observations are co-located, which can be achieved by putting them on the same platform. Also, the directional polarization instrument will benefit from co-location with the cloud imager.

- It is recommended to fly the Sentinel 5 Precursor mission in an afternoon Sun synchronous orbit, as also recommended by the CAPACITY study, for the following reasons:
  1. The UVN instrument in the afternoon orbit and the GOME-2 instrument in the morning orbit can provide information on the diurnal cycle of trace gases;
  2. The UVN in the afternoon orbit will continue the data record of OMI, whereas GOME-2 continues the record of the morning orbits from GOME and SCIAMACHY.
  3. For air quality forecasts the UVN observations are needed in the afternoon.

  Because especially the methane retrievals from the SWIR need very accurate cloud clearing, it is recommended to fly the Sentinel 5 Precursor mission within 10 minutes of the NPP/NPOESS mission, to allow the use of the VIIRS instrument for this purpose.

Bearing the cloud-free and L2 sampling statistics for various orbit combinations, together with other constraints on the mission, the following conclusions were reached with respect to each of the missions scenarios proposed for Sentinel 4/5:

- Geostationary and sun-synchronous polar orbit combination is now clearly the baseline that will be implemented, with Sentinel 4 / 5 providing additional instrumentation along-side Meteosat Third Generation (MTG) and Post-EPS (in 9:30 orbit similar to Metop). Provided pixel sizes are compliant with the MRD, the 9:30 orbit would not add significant additional sampling to that obtained from GEO, in the region where the latter makes observations (i.e. the European sector). Rather, the polar orbit will complement GEO by providing observations globally and by measuring species, which are not possible with GEO payload.

- A non-sun-synchronous constellation consisting of 3 satellites, with inclination 55 degrees separated in orbit phase evenly through the day, would generally provide sampling which is comparable to that of GEO in the mid-latitudes. It would provide almost identical probabilities of obtaining a single observation in a day, and only slightly fewer individual hourly samples within the day. The benefit over GEO would be that this sampling would be provided for all longitudes and include coverage of the tropics with slightly better sampling capabilities than an equivalent number of sun-synchronous orbits.
- Forming a Sun-synchronous constellation by combining observations from 9:30 and 13:30 sun-synchronous orbit leads to a substantial increase in the probability of obtaining compliant retrievals during a day, compared to 9:30 alone. Adding a further orbit with 15:30 *or* 17:30 local time further increases this probability though little further would be gained by adding both. For pixel sizes around 10km and field or regard of 20 km or larger, 3 sun-synchronous polar orbits give probabilities of one observation per day which are close to the NSS combination or GEO, particularly for TIR products, though generally the number of samples within a day is substantially smaller for regions where the NSS and GEO coverage is optimised. (However it is clear that sun-synchronous orbit provides far better sampling of the poles than the other options.)
- Given a realistic baseline for the Sentinel 4/5 that polar observations will be acquired from 9:30 and 13:30 orbit (Post-EPS and NPOESS), then it is clear from this analysis that the benefit of adding geostationary observations will be largely in terms of increasing the number of hourly samples acquired within the day, particularly for species for which sun-lit observations are required. GEO will not greatly increase the number of days on which a cloud-free observation is acquired. If this polar orbiter baseline is realised, then it seems sensible to optimise the GEO payload for species for which multiple samples during the day are a strong user requirement.

It is essential to have support of scientists throughout the design and build of the Sentinel 4, 5 and 5 precursor instruments. Using retrieval simulations and/or experience, scientist can assess the effects of instrument trade-offs, such as specific features of the Level 1B data on the Level 2 data, or when certain requirements are difficult to meet.

1 Introduction

This report presents the results of the ESA CAMELOT (Chemistry of the Atmosphere Mission concEpts and sentineL Observations Techniques). The CAMELOT study was conducted to develop the air quality and climate protocol components for the Sentinel 4 and 5 missions.

1.1 Background

In the next several decades a strong need is expected for operational *spaceborne* systems designed for atmospheric chemistry. First examples of this type of system within the 2010-2020 timeframe are EUMETSAT's Metop (with GOME-2 and IASI) and NPOESS (with OMPS and CrIS). However their set of observed chemical species is restricted, and, e.g., UV-VIS observations lack the necessary horizontal resolution for potential tropospheric applications.

In recent years, several ESA, EU and EUMETSAT activities have taken place to identify objectives and user requirements for operational atmospheric chemistry observations from ground and space.
The user requirements for space-borne atmospheric chemistry monitoring and possible mission concepts have been studied in the ESA CAPACITY (Operational Atmospheric Chemistry Monitoring Missions) study by a broad European consortium. The EU delivered the requirements for the GMES Atmospheric Services (GAS). These requirements are given for a system consisting of both ground based and remote sensing observations, which have been established by working groups of experts on these topics. Because the GAS user requirements are defined at this high-level, specific requirements for the space borne components cannot directly be derived from them.
The EUMETSAT Post-EPS Mission Expert Group has formulated geophysical observation requirements for the Post-EPS timeframe. The user requirements from Post-EPS expert group are largely consistent with those from the CAPACITY study.

The environmental issues identified in the CAPACITY study are:

- Stratospheric ozone and surface UV radiation,
- Air quality,
- Climate-chemistry interactions.

For each environmental issue three types of data usage were identified:

- Protocol monitoring (e.g. Montreal and Kyoto protocols, CLRTAP, EC directives),
- Near-real-time applications (e.g. NWP, air quality forecast),
- Environmental assessments (e.g. IPCC).

An application is defined by a combination of an environmental issue and a data usage type. For each of the resulting 9 application areas, quantitative geophysical observation requirements were established. Next, the check against the expected performance of the approved operational space-borne system for the next decade revealed the following main gaps:

I. High temporal and spatial resolution space-based measurements of tropospheric composition including the planetary boundary layer (PBL) for air quality applications;
II. 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;
III. High vertical resolution measurements in the upper troposphere/lower stratosphere (UTLS) region for stratospheric ozone/surface UV and climate near-real time and assessment applications.

Based on the CAPACITY results indicative mission concepts have been outlined to address the observational needs:

1. An air quality mission carrying a UV-VIS-SWIR spectrometer and possibly a TIR spectrometer. The spatial coverage and temporal resolution requirements imply the need of this payload complement on
    a. either a geostationary (GEO) satellite covering Europe and surrounding areas, plus a satellite on sun-synchronous low Earth orbit (LEO);
    b. or a constellation of three LEO satellites in inclined non-Sun synchronous orbit.

2. A climate monitoring mission carrying a UV-VIS-SWIR spectrometer and possibly a TIR spectrometer; due to large overlap of requirements this should be combined with the LEO (part of the) air quality mission.
3. A mission for stratospheric ozone and climate applications in the UTLS with a limb-sounding instrument either in the millimetre-wave or thermal infrared region.

It was recognized in the CAPACITY conclusions that the build-up of the observational capabilities could be done incrementally and that the lead-time for the LEO mission was probably shorter than that of the GEO mission. For the timeframe 2010-2020 an afternoon orbit was recommended for the LEO mission, in order to complement the Metop and NPOESS observations.

The recommendations of the CAPACITY have led to the definition of the Sentinel 4 and Sentinel 5 missions. The Sentinel 4 mission provides satellite observations from the geostationary orbit, focussing on air quality applications in Europe. The Sentinel 5 mission is a satellite in a polar LEO orbit aimed to address user requirements on global air quality, ozone layer and climate. The user requirements defined for the Sentinel 4 and 5 missions are based on the requirements from the CAPACITY study.

Since the start of the CAMELOT study in April 2007, the following programmatic decisions have been taken regarding the Sentinel 4 and 5 missions:

- The Sentinel 4 mission will be merged with the EUMETSAT MTG programme.
- The Sentinel 5 mission will be merged with the EUMETSAT Post-EPS programme.
- A precursor Sentinel 5 with launch date in 2014 was defined.

These decisions have significantly changed the perspective. In particular, the GEO-TIR component of the system concept for Sentinel 4 was abandoned due to partial overlap with the MTG-IRS instrument design at EUMETSAT. The latter is not being optimized for chemistry/air quality applications and so, the relevance of the CAMELOT study for the GEO-TIR component is out of scope and will not be considered in the CAMELOT study. The LEO-TIR requirements have been made consistent with the Post-EPS IRS requirements.

The overall goal of the CAMELOT study was to further develop the requirements for the Sentinel 4 and 5 missions for the air quality and climate protocol monitoring applications, including studies on alternative satellite constellations as recommended by CAPACITY. The CAMELOT study had the following main topics:

- The identification and quantification of meteorological and possibly other auxiliary data requirements and their priority compared to chemical data requirements;
- Trade-offs between different observation strategies (spectral ranges, polarisation, direction etc.) for aerosol and several gaseous species;
- The quantitative mapping of geophysical observation requirements onto instrument performance requirements and a review of the implementation-critical requirements
- Quantitative assessment of the requirements for spatio-temporal sampling taking into account the contamination of nadir-viewing observations by clouds;
- Contribution from the user's perspective to the trade-off between different orbit options.

1.2 Study Objectives

The key objective of the CAMELOT study was to contribute to the definition of the air quality and climate protocol monitoring parts of GMES Sentinels 4 and 5 within the time frame 2012-2020. In particular the MRD (Mission Requirement Document) user requirements Tables B1, B2 and C1 were in the scope of the CAMELOT study. These tables define the user requirements for air quality protocol monitoring, air-quality near-real-time applications, and climate protocol monitoring. The ozone layer user requirements (Tables A1, A2 and A3), the air quality assessment (Table B3) as well as the climate near-real-time and climate assessment (Tables C2 and C3) were out of scope for the CAMELOT study.

In the CAMELOT study, the following aspects have been studied

- Complementation of the geophysical observation requirements of the CAPACITY study by generation of meteorological and possibly other auxiliary data requirements and delivery time requirements;
- Contributions to trade-offs among different observation principles for several chemical species and parameters;

- Derivation of comprehensive instrument performance requirements from the geophysical observation requirements with previously identified observation principles, including in-depth study of implementation-critical requirements;
- Quantification of the effects of cloud interference as a function of geophysical and observational parameters;
- Optimisation of orbit scenarios and contributions to the trade-off between them;
- Support to parallel Sentinel 4 and 5 phase 0 and phase A system studies;
- Recommendations for changes and additions in the Mission Requirements Documents.

1.3 Overview of the study

As part of the CAMELOT study the following tasks have been performed:

- Task1: Preparation of geophysical scenarios for simulations;
- Task 2: Complementary observations and delivery requirements;
- Task 3: Retrieval simulations;
- Task 4: Assessment of cloud contamination;
- Task 5: Optimisation of mission scenario's;
- Task 6: Support to Sentinel 4 and 5 Phase 0 and Phase A system studies;
- Task 7: Conclusions and recommendations;

In Task 1 state-of-the-art chemistry transport and climate models have been used to produce four-dimensional datasets of trace gases and aerosols. From these datasets a set of scenarios has been selected that covers a wide variation of geophysical situations. The purpose of this dataset was to test retrieval simulations under different atmospheric conditions. In addition, a dataset of surface reflectivity at different wavelength and different spatial resolution has been produced.

In Task 2 the quantitative needs for auxiliary data for the Sentinel 4 and 5 missions have been investigated. Auxiliary data are all data needed in the Level 1B to Level 2 algorithms that do not originate from the instrument themselves, which may include for example pressure-temperature profiles, surface emissivity, boundary layer height, etc.. The second objective of Task 2 was to investigate the delivery requirements; i.e. the requirements on the maximum time between the observation and the availability of the data products. In this Task also an analysis has also been performed on the user requirements for the temporal resolution of satellite data for air quality applications.

The purpose of Task 3 was to derive the Level 1B requirements from the Level 2 user requirements for air quality and climate applications (tables B1, B2 and C1 of the MRD), using retrieval simulations. If more than one observational technique is available for a species (for example ozone can be observed in the UV and in the TIR spectral ranges), comparisons and trade-offs have been made between these techniques. For some species, also the combined retrievals using more than one spectral range have also been studied. Finally, the expected performance of the Sentinel 4 and 5 missions have been compared to the user requirements under different geophysical conditions and Sun-satellite geometries.

In Task 4 assessments have been made of cloud contamination. This task consisted of two main parts: (1) the collection and statistical analysis of a database of satellite observations of clouds, and (2) the calculation of the maximum tolerable amount of cloudiness for the retrieval of the species studied in Task 3.

In Task 5 orbit simulations have been performed to compare the different mission options. The orbit simulations take realistic cloud fields into account, by using the database that has been produced in Task 4. In addition the maximum tolerable amount of cloudiness has been taken into account for each species. By performing these orbit simulations in this way, statistical results can be derived on the chance of having an observation that meets the user requirements. These statistics have been calculated for different orbit options, including GEO, Sun-synchronous and non-Sun-synchronous orbits and their combinations.

In Task 6 responses have been prepared on specific questions from the industrial pre-Phase A studies for Sentinel 4 and 5. In addition, studies have been performed in support of the Sentinel 5 precursor mission, which has been defined during the project.

In Task 7 the conclusions and recommendations of the study have been derived.

2 Geophysical Scenarios for Retrieval Simulations

2.1 Introduction

The CAMELOT study requires geophysical scenarios of the atmosphere as input to the simulation of satellite retrieval of aerosol properties and trace gas concentrations. In accordance with the CAMELOT statement of work and project proposal, geophysical scenarios for retrieval simulations need to consist of a chemically and physically consistent set of geophysical input data for the year 2015, which is representative of the relevant geographical regions, e.g., the polluted regions of Europe, North-America, Asia, and the high-latitude regions which are important for climate applications and long-range transport. It includes temporal variations on diurnal and seasonal scale. The database is 3-D with horizontal and vertical resolution and includes scenarios for low and high concentrations. This input data set includes:

- aerosol and cloud parameter scenarios,
- physical atmospheric parameters such as temperature and humidity at several pressure levels,
- concentrations fields of trace gases foreseen as data products or influencing radiative transfer calculations: O_3, NO_2, SO_2, CH_2O, H_2O, CO, CH_4, HNO_3, N_2O_5, PAN
- spectral surface albedo, surface pressure and surface elevation.

The aerosol and trace gas profiles need to span the planetary boundary layer, including the free troposphere and the stratosphere. Physical consistency is best achieved using climate model output, representative for the next decade(s). Chemical consistency requires the use of simulations by a global chemical-transport model with a sufficiently complete chemistry scheme and driven by realistic emission distributions for all relevant compounds. Furthermore, preference should be given to simulations, which are traceable in the literature and as much as possible evaluated against observations. In addition, the requirements on diurnal time scales at high spatial resolution in the planetary boundary layer require the use of a regional chemistry transport model. This set of requirements made it necessary to use more than one model for the construction of the scenarios. A drawback is the necessity to harmonize the different model outputs per scenario / case. Note that even though each model includes its aerosol modules, the aerosol module of the climate model was chosen because it is considered more consistent with the physical climate parameters (e.g. hydrological cycle) than the aerosol module in an off-line global chemistry-transport model.

The following work has been performed as part of CAMELOT Task 1:

- analysis of simulation requirements and definition of the data set (Task 1.1), and the development and content of the database containing
- physical atmospheric parameters such as temperature and humidity at several pressure levels (Task 1.2);
- aerosol and cloud parameter scenarios (Tasks 1.3 and 1.4);
- the ‘trace-gas vertical profiles data base’ that was developed for application in Task 3 (retrieval simulations). (Task 1.5);
- The development of a surface reflectance database spanning a wavelength range from the UV to the TIR. (Task 1.6);

Details on the approach and results have been provided in report RP-CAM-FMI-030. The database is available to CAMELOT project team member through the CAMELOT coordinator at KNMI.

2.2 Analysis of simulation requirements

A questionnaire on scenario requirements for 2015, sent to all CAMELOT partners, and ensuing discussions, lead to the formulation of the set of scenarios used in CAMELOT (TN-CAM-FMI-006). The selected locations are presented in Table 1.1 and shown in the map of Figure 2-1. These scenarios are based on IPCC and recent developments as explained in RP-CAM-FMI-0030.

2.3 Models used to generate the CAMELOT database.

Three models were used to generate the CAMELOT database. ECHAM5-HAM and CHIMERE data have been provided with the full model spatial and temporal resolutions, whereas for TM4 selected average profiles have been made available. These are fixed parameters and cannot be changed to smaller spatial resolution. CHIMERE model runs are made to match the retrieval resolution to the model resolution, which is comparable to the pixel size of most instruments. Table 2-1 summarizes the resolution and data coverage for each model.

Table 2-1. The basic set of 16 selected cases that are considered representative for CAMELOT retrieval simulations under a wide range of conditions.

Nr.	Selected case	Latitude [-90°, +90°]	Longitude [-180°, +180°]	Month
1	Europe background	45	2	June
2	Europe polluted	51	7	June
3	China polluted	31	115	June
4	Pacific polluted	31	140	March
5	US East coast polluted	40	-75	June
6	Tropical background	-10	-180	October
7	Tropical BMB (land)	5	20	January
8	Tropical BMB (ocean)	5	5	January
9	Tropical dust (land)	20	-10	June
10	Tropical dust (ocean)	20	-30	June
11	Subtropical background	-30	90	October
12	Stratospheric intrusion	40	-73	28 January
13	Polar North Sodankyla	68	26	June
14	Polar South Marambio	-64	57	October
15	Melting permafrost Siberia	67	146	June
16	Volcanic (Etna)	38	15	July

Tools have been developed for CAMELOT to extract any desired profile with a resolution of 6 hours for ECHAM and a resolution of 1 hour for CHIMERE. Monthly averaged profiles and their standard deviations were computed from the database as examples and have been made available graphically in digital form.

In summary:

- ECHAM5-HAM delivers 6-hourly resolution with spatial resolution at T42 (grid interval approximately 300 km in horizontal at the equator) in the model grid (so-called Gaussian grid) at 19 altitude levels. The model top is at 10 hPa (approximately at 30 km height) for 2015.
- TM4 delivers selected time averaged profiles with spatial resolution of 3 x 2 (lon x lat) degrees, with 25 vertical levels up to 0.1 hPa, for 2030.
- CHIMERE delivers hourly resolution for 13x13 km^2, over Europe for June 2006.

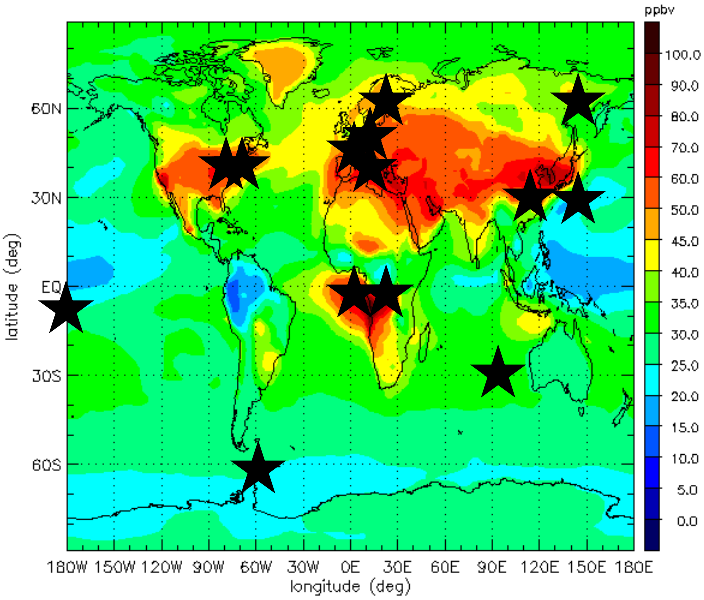

Figure 2-1. The geographic spread of the 14 selected locations. The underlying map shows the surface ozone concentrations (in ppbv) for June 2000 simulated using TM4.

Table 2-2. Resolution and data coverage of the models used for the ONTRAQ geophysical scenarios

MODEL	**ECHAM5-HAM**	**TM4**	**CHIMERE**
Time resolution	6 hours	Monthly average	1 hour
Spatial resolution	T42 (approx. 300 km at equator)	3 x 2 (lon x lat) degrees	13x13 km^2
Vertical resolution	Gaussian grid, 19 levels	25 hybrid levels	8 hybrid levels
Highest level	1 hPa	0.1 hPa	500 hPa
Coverage	Global	Global	North-West Europe
Period	2015, whole year	2030	June 2006
Availability	HD sent to KNMI	Datasets on ftp	Full datasets on ftp

2.3.1 Atmospheric physical and aerosol parameters

2.3.1.1 Background

Physical atmospheric parameters (temperature, humidity, clouds and aerosols) in 2015 can only be predicted through global scale Earth System Models (ESM) using future emission databases. While it is common today to consider climate change scenario data for atmospheric parameters such as temperature, precipitation, wind, etc. in the global change context, as yet it is very uncommon to consider such data for aerosols. Only during the very recent years size resolving models of aerosol microphysics have become mature enough to be included into ESMs. Thus, generation of a database of future atmospheric aerosols in the CAMELOT project is a true innovation, and probably one of the very first such endeavours worldwide.

2.3.1.2 Climate scenarios

Realistic climate scenarios form the basis of the CAMELOT database of physical atmospheric quantities. Here, efforts of the Intergovernmental Panel on Climate Change (IPCC) have been utilized. IPCC future climate scenarios are based on hypothetical scenarios of CO_2 and other greenhouse gas emissions under different socio-economic assumptions. For CAMELOT, the IPCC scenarios (IPCC 2000) A2 (heterogeneous world, rising population, slow technological change), A1B (rapid growth of world economy and population, advent on new and more efficient technologies, balanced use of fossil and renewable energy sources) and B1 (rapid development towards environmentally friendly technologies) were considered. In the A2 (A1B, B1) scenario, the atmospheric CO_2 concentration increases from the pre-industrial value of 280 parts per million by volume (ppmv) to 550 (700, 830) ppmv by the end of the 21st century.

2.3.1.3 The MPI-M climate model

The coupled atmosphere-ocean general circulation climate model of the Max Planck Institute for Meteorology (MPI-M), Germany, was used to provide scenarios (i.e. the necessary boundary conditions for the CAMELOT simulations) for the period 2000 - 2015. The MPI-M climate model consists of two components: the atmosphere and land surface model ECHAM5 (Roeckner et al. 2003 and 2006a) and the ocean model MPI-OM (Jungclaus et al. 2006). The horizontal resolution of the atmosphere model in the runs for the AR4 was 1.875 degrees (grid distance of about 200 km at the equator) while the ocean model resolution was 1.5 degrees (about 160 km). The models contain processes that are resolved by the grid, as well as unresolved parameterized processes, which are important for describing the transport of energy, momentum and water in the Earth system (Roeckner et al. 2006b).

2.3.1.4 The aerosol scenarios

The IPCC simulations by the MPI-M do not contain aerosol scenarios, which were successfully produced within the CAMELOT project. The necessary elements for the aerosol scenario production are as follows: a size resolving model of aerosol microphysics, a model for natural primary aerosol emissions, and scenarios for primary anthropogenic aerosol emissions for the year 2015 in accordance with the IPCC storylines A2, A1B and B1.

Aerosol microphysics

A version is available of the ECHAM5.3 atmospheric model that is coupled with the aerosol model HAM (MPI-M Hamburg Aerosol Model; Stier et al. 2005). The HAM model describes the atmospheric aerosol microphysics using a modal representation with 7 aerosol size modes for 5 chemical components (Vignati et al. 2004). The HAM model is capable of describing the aerosol microphysical processes in the atmosphere (nucleation, condensation, deposition, and coagulation), atmospheric transport of aerosols, and interactions of aerosols with solar radiation and long wave radiation emitted by the Earth system. This model is, however, computationally extremely demanding, due to a very large number of variables in the aerosol model to be computed and stored in the computer's run-time central memory. Therefore the aerosols were not a routine part of the IPCC 4AR production runs. Even in the CAMELOT simulations, which were considerably shorter than the IPCC AR4 simulations of MPI-M, it is only possible to couple the HAM model with an ECHAM5 model version with a lower resolution than that used for the IPCC AR4 simulations at MPI-M.

Model for natural primary aerosol emissions

The HAM model also includes model state dependent parameterization of natural primary aerosol sources. The natural aerosol emissions are thus fully consistent with the model dynamics (i.e. model surface wind and boundary layer turbulence), first, over oceans where the model surface winds generate waves which upon breaking produce sea spray aerosol, and, second, over bare land and desert areas where mineral dust aerosol is generated through the model surface winds lifting dust into the atmosphere.

Scenarios for anthropogenic primary aerosol emissions

The standard ECHAM5-HAM model includes primary anthropogenic emissions for black carbon (BC) and organic carbon (OC) due to use of bio fuel and fossil fuel based on the AEROCOM2000 (Dentener et al. 2006) emission inventory. Formally these emissions are valid for the year 1996. Scenarios for these same aerosol emissions for the year 2030 are estimated in Streets et al. (2004). Emissions for 2015 were simply interpolated from the emission data for 1996 and 2030.

Open burning emissions of BC and OC for 2015 are scaled from the AEROCOM2000 wildfire emissions, separately for the B1, A1B and A2 scenarios. In each experiment, the same emissions for SO_2 and di-methyl-sulphide (DMS) were applied. In addition, a control experiment (see below) was conducted for evaluation and quality assurance purposes, and that experiment makes use of the AEROCOM2000 emissions as such.

2.3.1.5 The CAMELOT procedure for generating scenarios of physical parameters and aerosols

The atmospheric (physical) parameters were generated in the CAMELOT project using the ECHAM5.3 atmospheric general circulation model. Sea surface temperature (SST) and sea ice coverage, i.e. the boundary conditions for the atmospheric climate model simulations, were taken from the corresponding MPI-M archive of IPCC-AR4 scenario products. Generation of these products employed the coupled ECHAM5-MPI-OM climate model.

Each experiment was started from 1 Jan 2010 with its own SST, sea ice coverage, greenhouse gas concentration and AEROCOM2000 (standard) emissions of BC and OC due to bio fuel and fossil fuel as well as open burning. Each experiment was run with the above boundary conditions until 31 Dec 2013 so as to let the climate model system to spin down to the attractor limited by the provided AR4 boundary conditions. The experiments thus follow closely and consistently the IPCC 4AR scenarios produced by the MPI-M. Each experiment continued from 1 Jan 2014 as above, but with the estimated bio fuel, fossil fuel and open burning emissions of BC and OC for 2015 according to A2, A1B and B1 scenarios, respectively. The control experiment continued with the standard AEROCOM2000 emissions. These "own emissions" were introduced already in the beginning of the year 2014 so as to let the coupled atmosphere – aerosol model to adjust to the abruptly changing new emissions before the actual target year of 2015. Experiments were stopped at 31 Dec 2015.

2.3.1.6 Geophysical and aerosol data set created for CAMELOT

The CAMELOT model output is a one-year global data set of aerosol scenarios for 2015 at the model resolution T42 (grid interval approximately 300 km in horizontal at the equator) in the model grid (so-called Gaussian grid) at 19 vertical levels. The model top is at 10 hPa (approximately at 30 km height) and the time interval of the global fields is six hours. A parameter list of the data is provided in Appendix A. Probably the most relevant ones are the profiles of air temperature, specific humidity, cloud water and ice mixing ratio, aerosol mass mixing ratios of sulphate, black carbon, organic carbon, sea salt and mineral dust in the accumulation, Aitken and coarse modes for both soluble and insoluble modes, as well as aerosol number mixing ratios in accumulation, Aitken and coarse modes for soluble and insoluble modes. There are profiles of 52 parameters thus to be studied, for each of the IPCC scenarios A2, B1 and A1B, as well as a control experiment (referred to as 20C).

2.3.1.7 Data quality control

A large amount of qualitative diagnostics of the database has been performed, such as visual inspection of vertical profiles, time series, as well as maps of integral quantities related to various model output parameters. Some anomalies are found but the limitations of the CAMELOT project do not allow for exhaustive quality control of the database.

2.3.2 Trace gas scenarios

2.3.2.1 Emission scenarios

Expectations for future changes in the global atmospheric composition were derived following the approach by Dentener et al. (2006) combining expectations for energy use (IPCC-SRES, 2000) and air quality legislation (Amann et al., 2004; Dentener et al., 2005) to deal with future emission uncertainties. For the physical and aerosol scenarios, first the year 2000 was examined as baseline year for which present-day atmospheric models, driven by present-day emission estimates on high spatial resolution, were evaluated. Next, future emission scenario simulations were compared against the year 2000 baseline. Future emission estimates are typically based on regional scaling of present-day emission estimates. For this purpose, the world is divided into 11 land regions and the oceans.

Dentener et al. (2006) present three emission scenarios for the year 2030. For CAMELOT the intermediate ‘CLE (Current Legislation)’ scenario was used, which reflects the implementation of current air quality legislation around the world. The CLE scenario is based on the moderate IPCC SRES B2 energy scenario. The CAMELOT study was not intended nor funded to establish future emission and concentration scenarios, and therefore the study depends on the scenarios that are available and these have been used.

Dentener et al. (2006) present ensemble model simulations (including TM4 simulations, see below) for the year 2030 from which global surface ozone is calculated to increase globally by 1.5±1.2 ppb (CLE), using the ensemble mean model results and associated ±1σ standard deviations. In the CLE scenario CO emissions are projected to decrease globally, NMVOC emissions remain almost constant and NO_X emissions are projected to increase globally by ~12% with respect to the base year 2000.

2.3.3 TM4 global chemistry transport model

The off-line TM4 chemistry-transport model has a regular longitude–latitude spatial grid, and hybrid σ–pressure layers in the vertical. It is driven by six-hourly meteorological fields from the European Centre for Medium Range Weather Forecast (ECMWF) operational data. These fields include global distributions for horizontal wind, surface pressure, temperature, humidity, liquid and ice water content, cloud cover and precipitation. Key processes included are mass-conserved tracer advection, convective tracer transport, boundary-layer diffusion, photolysis, dry and wet deposition, as well as tropospheric chemistry including non-methane hydrocarbons. The anthropogenic emission distributions applied here are described in Stevenson et al. (2006). TM4 spatial resolution is 3 x 2 (lon x lat) degrees, with 25 vertical levels up to 0.1 hPa. A mass-conserving pre-processing of the meteorological input is applied for TM4.

The present-day short-term and spatial variations are considered robust and most relevant for the retrieval sensitivity simulations in CAMELOT. A set of cases, mainly defined by geographic location and temporal variations has been selected for use in the retrieval studies. These cases can be considered adequate for a satellite mission in the 2015 timeframe.

2.3.4 CHIMERE regional chemistry-transport model and the Summer 2006 scenario

CHIMERE is a three-dimensional Eulerian chemistry-transport model. It has been applied over different domains, from the urban to the continental scale. The CHIMERE model is part of the national air pollution forecasting system in France (Prev'Air). It has been intercompared to other CTMs over several European cities (Cuvelier et al., 2007). For the CAMELOT study, we use a continental configuration over western Europe with a horizontal resolution of 0.5 x 0.5 degrees. Model version is CHIMERE 2006a. The applied time step is 10 minutes. Model output is hourly. The model vertical domain is limited to the planetary boundary layer and lower troposphere up to ~ 600 hPa (or 4 km). We use a simulation for June 2006 for which trace gas fields were stored on hourly basis. June 2006 was a relatively warm. It is assumed that the levels of air pollution that are simulated for this month may serve as a possible scenario for (future) polluted summer periods over Western Europe. It is probably a relatively pessimistic scenario because most projections foresee emission reduction over Western Europe in response to current legislation for air quality.

2.4 Surface albedo scenarios

The CAMELOT study requires atmospheric scenarios including information on surface reflectance to assess the performance of the satellite retrieval algorithms. Surface albedo data ranging from the ultraviolet wavelengths (~300 nm) to the thermal infrared (~15 μm) are needed. The following primary sources of albedo and BRDF data were considered for the construction of the surface albedo database:

1. GOME: http://www.temis.nl/data/ler.html
2. MODIS: ftp://modis-atmos.gsfc.nasa.gov./L3LandSurfaceProducts/Data/
3. AVIRIS: http://speclab.cr.usgs.gov/spectral-lib.html
4. ASTER: http://speclib.jpl.nasa.gov/
5. POLDER BRDF: by request from François-Marie Bréon (fmbreon@cea.fr)

The reflectance databases are used for the different scenarios according to land use provided by the IGBP (International Geosphere-Biosphere Program) land cover classification, which includes 17 classes. These are 11 natural vegetation classes, 3 developed land classes (one of which is a mosaic with natural vegetation), permanent snow or ice, barren or sparsely vegetated, and water. These classes are shown in Figure 2-2 and are listed in Table 2-3. The resolution of this dataset is 0.05 degrees, which corresponds to approximately 5600 meters.

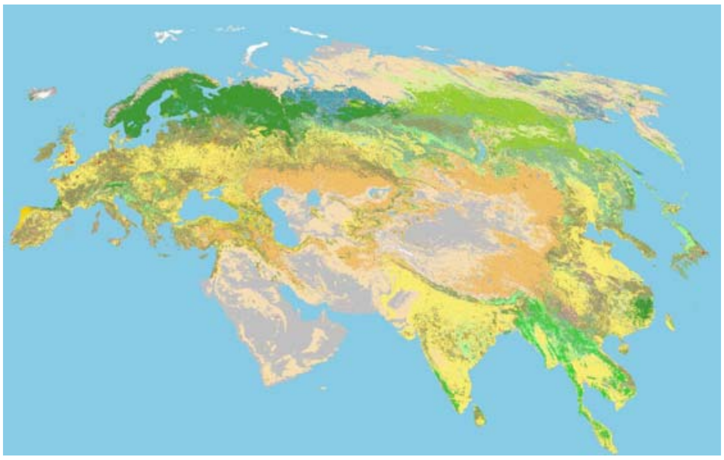

Figure 2-2. IGBP land cover classes for Europe and Asia.

Table 2-3. IGBP land cover classes

MOD12C1 Land_Cover_Type_1 (IGBP)		
Land Cover	Class	Color
Fill Value	255	
Water	0	
Evergreen Needleleaf Forest	1	
Evergreen Broadleaf Forest	2	
Deciduous Needleleaf Forest	3	
Deciduous Broadleaf Forest	4	
Mixed Forest	5	
Closed Shrubland	6	
Open Shrubland	7	
Woody Savannas	8	
Savannas	9	
Grasslands	10	
Permanent Wetlands	11	
Croplands	12	
Urban and Built-Up	13	
Cropland/Natural Vegetation Mosaic	14	
Snow and Ice	15	
Barren or Sparsely Vegetated	16	
Unclassified	254	

Reflectance spectra were calculated for the scenarios over land (see Table 2-1) and the reflectance spectra for the IGBP land cover classes in all seasons with and without snow from GOME and MODIS. Winter is referred to as December to February, spring as March to May, summer as June to August and fall as September to November. GOME provides the Lambert-equivalent reflectivity (LER) and MODIS white-sky albedo. These are not exactly the same and therefore spectra from different instruments have not been combined. The albedo/BRDF of the ocean surface varies with atmospheric conditions, like wind speed and direction, and with oceanic parameters such as sea state, the occurrence of phytoplankton and dissolved organic matter, and also with the viewing geometry. Thus, we recommend the use of validated models for the calculation of ocean surface albedo/BRDF.

2.4.1 GOME data

The GOME global dataset consists of monthly minimum LER values (Koelemeijer et al., 2003). These data cover the period from June 1995 to the end of the year 2000 with a spatial resolution of 1° x 1° and provide LER for eleven 1-nm-wide wavelength bins centred at 335, 380, 416, 440, 463, 494.5, 555, 610, 670, 758, and 772 nm. Errors in the derived LER values are mainly caused by errors in radiometric calibration of GOME and errors caused by residual cloud contamination. Moreover, the assumption that minimum LER values represent aerosol-free conditions is not always valid.

The IGBP data was used to locate 1° x 1° regions where only one land cover class was present, and determined from the GOME LER data the mean LER for different land cover classes for these sample regions. The number of locations for different land covers classes varied from 10 to 50. The standard deviation of the land cover specific spectra was determined from the variation of the measurements in the selected locations. GOME data was separated into snow and snow free cases based on the reflectance in the smallest channel (335 nm). If reflectance was over 0.1 in that channel, the measurement was categorised to include snow.

2.4.2 MODIS data

The MODIS albedo data base constructed by Moody et al. (2005, 2007a, 2007b) provides white-sky albedo values for the first seven MODIS bands centered at 470, 550, 690, 860, 1240, 1640, and 2100 nm, and they are classified according to their land cover types for 16-day periods from a 5 year data set (2000-2004). Seasonal mean values were calculated by combining 5 or 6 periods. The data provided by Moody contained the albedos and standard deviations for all land cover types with and without snow. Data was also provided for the Southern and Northern hemisphere separately. Snow-free data were available for all seasons, but obviously snow-cover related data were available only for winter months.

2.4.3 AVIRIS data

For the longer wavelengths we chose to use the AVIRIS data from the USGS database. This data set contains six spectra measured from an airplane. The downside of the dataset is that the AVIRIS spectra cover only wavelengths up to 2.5 micrometers and it does not contain information on the accuracy of the measurements. For the scenarios, we calculated the standard deviation based on the differences between the land cover classes inside the scenario pixel. In view of the limited number of the AVIRIS spectra available for the different land cover classes it was assumed that one tree type represents all the different needle leaf forest types. Similarly, a single spectrum was used for all broadleaf forests. For the Urban, Cropland and Bare land cover types there was no data available from AVIRIS.

2.4.4 ASTER data

For the thermal infrared, ASTER data were used which cover wavelengths from 0.3 to 14 micrometers. The ASTER spectral data library contains four usable spectra for vegetation (conifer, deciduous trees, green and dry grass). In addition, we calculated four typical spectra: The soil spectra is averaged from 5 measurements: black loam, gray silty clay, grey calcareous silty soil, red orange sandy soil and very dark grayish brown silty loam. The urban spectrum was obtained by averaging 4 measurements: asphalt, concrete, galvanized steel and tar paper. The rock spectrum was obtained by averaging 5 measurements: basalt, diabase, granite, grey limestone and white sandstone. The desert spectrum was obtained by averaging 2 measurements: yellowish loamy sand and gypsum sand.

ASTER data sets are not recommended to be combined with the other data sets because they ASTER data are based on point measurements which are not in general applicable to satellite retrievals (Liang, et al., 2002). They do not include information about seasonal variation in vegetation, and combining of vegetation and soil types for a “typical” combination requires lots of assumptions (e. g. the spectra used in the averaging were selected from a limited data set, thus the resulting spectra may not be representative globally) and thus the uncertainty will be very large and reflectance in the data base (bidirectional/directional (10 degree) hemispherical reflectance) is not exactly the same as albedo or BRDF. This data set is reproduced from the ASTER Spectral Library through the courtesy of the Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California. Copyright 1999, California Institute of Technology.

2.4.5 BRDF data

The directional signatures used in this project were derived from the CNES Parasol instrument. More information about the BRDF data derived from POLDER has been published by Bacour and Bréon (2005) and Maignan et al. (2004). The BRDF is expanded into a linear sum of terms (the so-called kernels), characterizing different scattering modes. The superposition assumes that these modes are either spatially distinct within the scene viewed with little cross coupling, physically distinct within a uniform canopy with negligible interaction, or empirically justified. The resulting BRDF model is called a kernel-based BRDF model (Lucht et al., 2000b). For the BRDF data we deliver typical BRDF shapes as a function of IGBP surface type and Normalized Difference Vegetation Index (NDVI). Bréon mixed data from the northern and the southern hemisphere, as well as from tropical regions. Data for different seasons were mixed as well; therefore NDVI is a better parameter for the yearly cycle of vegetation. The data include two parameters k1/k0 and k2/k0 for each wavelength/IGBP class/NDVI class and the BRDF shape is 1 + k1/k0 F1(thes,thev,phi) + k2/k0 F2(thes,thev,phi), where thes, thev and phi are solar zenith, view zenith and relative azimuth angles, respectively, F1 and F2 are a-priori kernels based on either physical or empirical considerations, and k0, k1 and k2 are free parameters to be inferred from the measurements. Bréon has used the Rossthick-Roujean (with hotspot) three-parameter semi-empirical model (Bacour and Bréon, 2005) while people working with MODIS data have used the RossThick-LiSparse (reciprocal) model (Lucht et al., 2000). The resulting shapes from these two models are fairly similar, but the k1 and k2 proportions may differ because the kernels are slightly different. Crystal Schaaf from Boston University, USA, and her team have provided MODIS based BRDF data which can be downloaded from their website, see section 2.8 for more information.

2.5 Albedo/BRDF over ocean

The ocean surface albedo was calculated for a scenario with the Coupled Ocean and Atmosphere Radiative Transfer (COART) model. This model can be used online at http://snowdog.larc.nasa.gov/jin/rtset.html.

2.6 Chemical Transport Model Simulations

The ECHAM-HAM simulations show that experiments with future emissions do not significantly differ from the control experiment (emissions of AEROCOM2000). In other words, variability of atmospheric parameters (diurnal, synoptic, annual, …) seems to be larger in each experiment than the differences between the experiments with different emissions. This aspect is illustrated in Figure 2-3, and it may be good news for the need of robustness of retrieval algorithms in future atmospheric conditions.

Similar observations were made from the TM4 simulations. The calculated changes are significantly smaller than seasonal and even diurnal variations in trace gas concentrations as well as typical geographical variations over the world. For example, one may compare the 1.5 ppb overall increase in surface ozone (Dentener et al., 2006) with the 20-80 ppb range of (present-day) surface ozone levels in the chosen geophysical scenarios, and the projected increase of 1.7 ppb in global CO at 500 hPa (Shindell et al., 2006) with the range of 70–150 ppb for CO concentrations at this level in the chosen scenarios (see chapter 2 for the different geophysical scenarios).

The ECHAM-HAM results show that anomalous natural emissions of mineral dust were detected. Downstream of the Saharan desert over the Atlantic Ocean just off the African coast (21N, 31W) values of atmospheric optical depth of ~13 occur (c.f. panel (f) in Figure 2-3). This is likely due to a gross over estimation of natural emissions of desert dust. These events are however very short lived and normal levels of aerosol are quickly reached due to deposition of excess aerosol from the atmosphere, as modelled in the HAM.

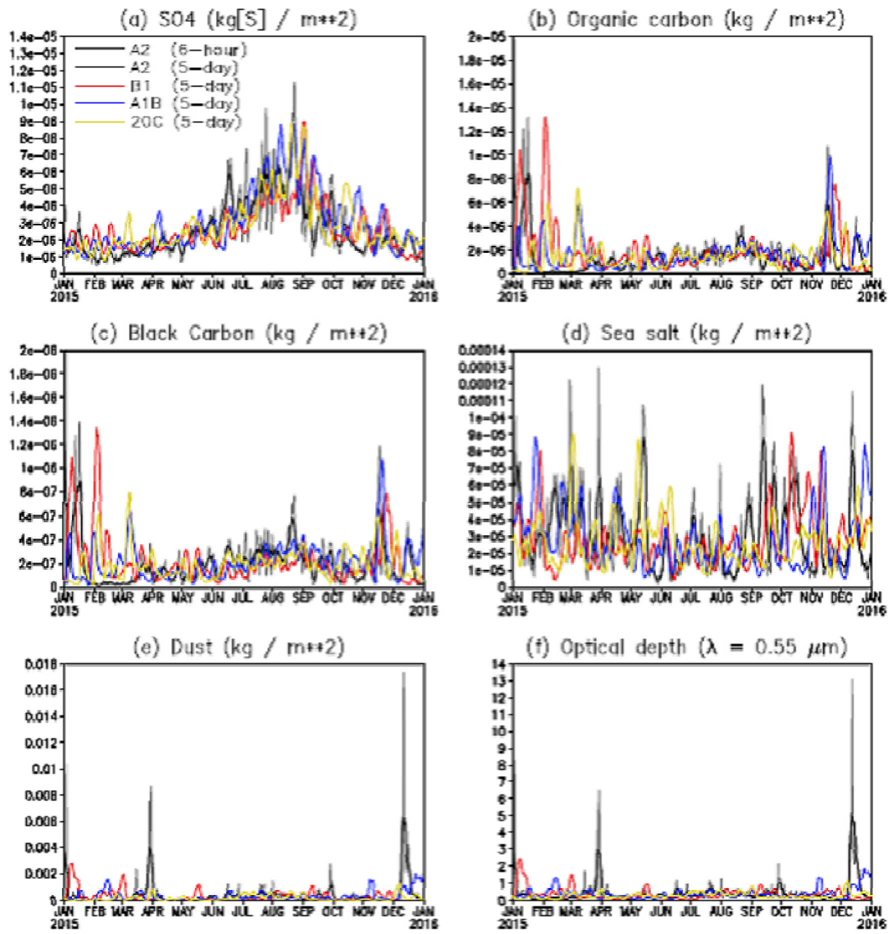

Figure 2-3. Time series of vertical integrals of (a) SO_4 aerosol amount, (b) organic carbon, (c) black carbon, (d) sea salt, (e) dust, and (f) aerosol optical depth for the grid point corresponding to the Atlantic Ocean at 20.9 N, 30.9 W. The grey lines give the values for the A2 scenario at the original 6-hour resolution of the data set. The black, red, blue and yellow lines are corresponding five-day running mean values for the A2, B1, A1B and 20C emission scenarios, respectively. Note the peaks in panel (e) and (f).

2.6.1 ECHAM-HAM results

For each of the 4 scenarios, and each of the 16 locations, there are profiles of 52 parameters (e.g. air temperature). The selected cases agreed upon by the CAMELOT project team contain thus in total 3120 profiles. Each profile is generated from the 6 hourly model data over a period of one month (about 120 profiles). Users have, of course, access to the instantaneous profiles all over the globe, and the data volume from their perspective is thus enormous. A representative set of 52 profiles (European Background (46.0 N, 2.8E) A2 scenario for June 2015) out of the 3120 profiles of the CAMELOT special cases has been provided in the Task 1 report RP-CAM-FMI-030. Additionally, time series of vertical integrals of SO_4 aerosol amount, organic carbon, black carbon, sea salt, dust, and aerosol optical depth for the grid point corresponding to the European Background case were presented. Geographical maps of annual-mean horizontal distribution of simulated aerosol optical depth at λ = 0.55 µm, for the A2, B1, A1B and 20C (i.e., the control experiment) emission scenarios are depicted in Figure 2-4. The global mean values are given in parentheses in the panel captions. Figures of all scenarios have been produced and are available in electronic form.

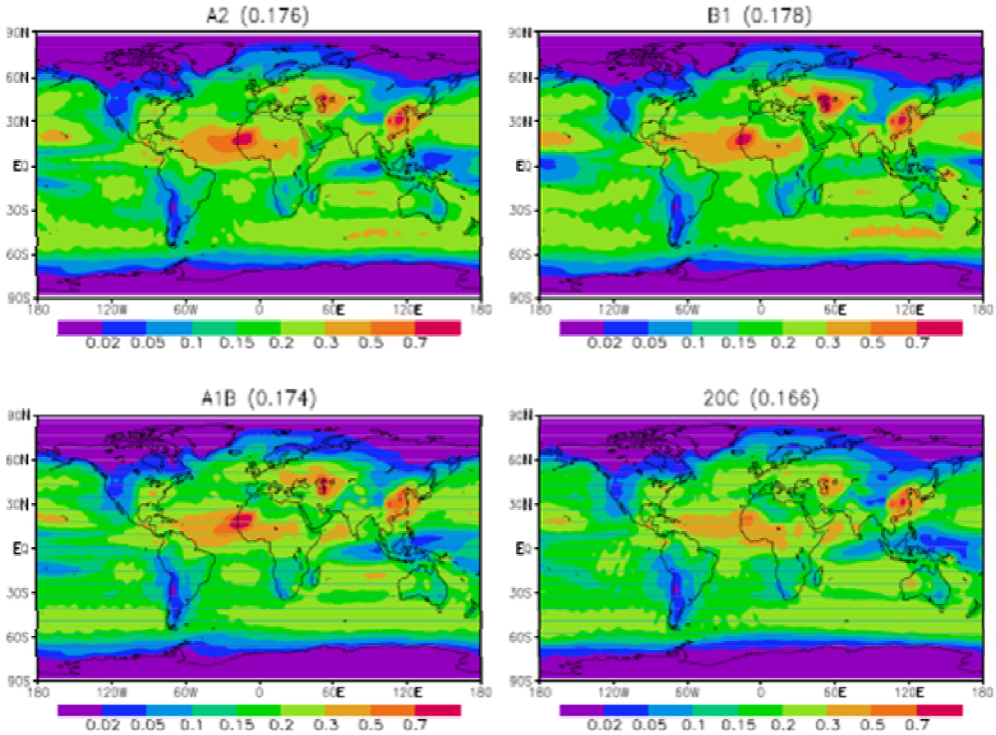

Figure 2-4. Annual-mean horizontal distribution of simulated aerosol optical depth at λ = 0.55 µm, for the A2, B1, A1B and 20C emission scenarios. Global mean values are given in parentheses in the panel captions.

2.6.2 Trace gases: TM4 and CHIMERE

Projected decadal changes in the atmospheric composition between 2030 and 2000 are typically small in comparison to the spatio-temporal variability in atmospheric composition on time scales from hours to seasons and from one place to another. In order to support CAMELOT retrieval studies under a wide range of conditions, monthly-mean vertical profiles have been extracted at 16 representative locations around the world for selected months. Furthermore, zonally averaged profiles and standard deviations based on longitudinal variations have been calculated for the latitude band and month of each case. The in CAMELOT agreed months that have been chosen for the selected locations are 'June' for the Northern Hemisphere and 'October' for the Southern Hemisphere. For some cases we decided to deviate from these standard selected months, as explained below. For the European cases additional information on the diurnal variation – daily means and standard deviations based on the diurnal cycle of the trace gases – is added using CHIMERE model output, which is also on higher spatial resolution of 0.5 x 0.5 degrees. A selection of results was presented in RP-CAM-FMI-030. As an example, Figure 2-5 shows the TM4 calculated global distribution of the annual-mean tropospheric NO_2 columns for the year 2000 and for 2030 in the CLE scenario. Projected increases in NO_x emissions over East and South Asia between 2000 and 2030 are on the order of 10 to 15%.

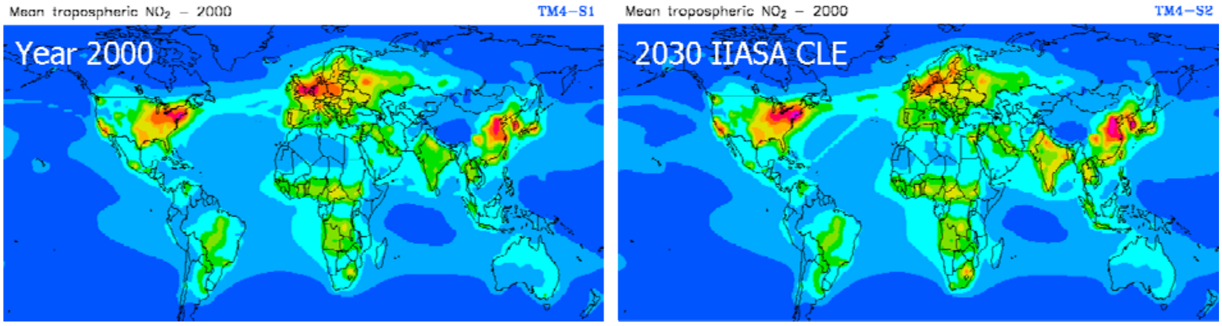

Figure 2-5. Annual-mean tropospheric NO_2 column density calculated with TM4. Left: Year 2000 (run S1); Right: CLE scenario for 2030 (run S2). (Noije et al., 2006; van Noije (personal communication, 2007).

2.6.3 Surface albedo results

Representative examples have been presented in the Task 1 report RP-CAM-FMI-030. Figure 2-6 depicts an example that shows that spectra from different instruments can have significant differences. Snow can alter the spectrum very much, especially in the wavelength region below 1 µm.

Similar data sets are ready for all the IGBP land cover classes for each season from GOME and MODIS. In addition we calculated the values with or without snow. AVIRIS data is available for 11 land cover classes in the summer.

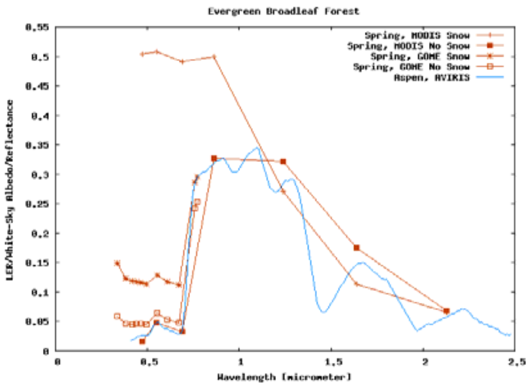

Figure 2-6. Reflectance spectra for evergreen broadleaf forest in spring from GOME (white squares=without snow, stars=with snow), MODIS (dark squares=without snow, crosses=with snow) and AVIRIS (blue).

2.7 Data base description

2.7.1 Physical and aerosol data base and the user interface

The CAMELOT database is provided as NetCDF files, including in total 144 files (3 files per month for the 12 months of the year for the 4 emission scenarios A2, B1, A1B and control). The data volume amounts to slightly over 200 GB. The data are split into three files per month to keep the file size manageable (i.e., < 2 Gb) also for systems without Large File Support (LFS). The files can be read by any standard tool designed to handle NetCDF data. For example, in Unix/Linux the contents can be browsed using the ncview–software. The data can also be read by Fortran90 programs (e.g. http://www.unidata.ucar.edu/software/netcdf/docs/netcdf-f90). The database has been delivered to KNMI as CAMELOT coordinator on an external hard disk and will be made available by KNMI to the users on an ftp site.

2.7.2 Trace gas data base

The trace gas database consists of two components; a small selection of data (~ 200 kb) and a large complete data set (~ 500 Mb).

The first and small data set component consists of 32 ASCII files containing vertical profiles. There are two files for each of the selected cases in Table 2-1. The first set of files, e.g., 'case1_European_background.dat') contains, for each case, monthly-mean vertical profiles at (lat, lon) based on TM4 (Year 2000). The second set of files, with extensions ('_zonal.dat'), contains for each case the zonal average monthly-mean profiles for the latitude band of the case, as well as the standard deviation of the zonal mean based on longitudinal variation along the latitude band.

For cases 1 and 2 the ASCII files contain in addition:

- the recommended combined monthly-mean vertical profiles at (lat, lon) based on TM4 (June 2000) + CHIMERE (20 June 2006)
- the daily-mean vertical profiles at (lat, lon) based on CHIMERE (20 June 2006)
- standard deviations of daily-means based on CHIMERE hourly model output data (25 concentrations)

The second and largest data set component consists of the full 2- and 3-dimensional data sets in netCDF format from which the 16 cases were selected as well as some IDL reading/plotting routines for these data sets. The IDL routines read the netCDF data files. New ASCII-type of files can easily be created using the accompanying IDL routines.

This full data set allows the user to switch between the emission scenarios from 2000 to CLE 2030. Furthermore, with this data set it is possible to select zonal means and standard deviations for other latitude bands than those that have been selected for the 16 locations. Finally, the 3-D model data is delivered for each month of the year. This allows the user to get information on seasonal variations in the trace gas profiles, e.g., at the 16 selected locations.

Concerning the constructions of new cases (ASCII files) for Europe that are similar to cases 1 and 2 using the combination of TM4 and CHIMERE model output some additional remarks are needed. First, CH_4 levels in CHIMERE are significantly lower than in TM4. In fact, CHIMERE methane surface concentration levels are prescribed (at too low levels) and not calculated from simulations with explicit methane emissions. Therefore, it is recommended NOT to replace TM4 methane profile with the CHIMERE methane profile for the lowest layers (below ~600 hPa). Secondly, the CHIMERE simulation did not output N_2O_5, even though nighttime chemistry involving e.g. NO_3 and N_2O_5 is fully taken into account in CHIMERE. Therefore, similar as for methane the TM4 N_2O_5 profile should be kept for the layers below ~ 600 hPa.

The directory and file naming structure of the trace gas database is straightforward and kept fairly simple: For details see RP-CAM-FMI-030.

2.7.3 Surface albedo data base

The constructed database includes data from GOME, MODIS, AVIRIS and ASTER and it is available at KNMI. Each of these data sets has their own folder and data format. In addition, the data for the scenarios over land have been categorised by the instruments, pixel size (5, 10, 20, 40 and 80 km), season and snow cover, and file names are based on them: "China_polluted_10km_fall_mean_no_snow_GOME.dat". Scenario folders also include satellite pictures and IGBP maps of the scenario area. The different pixel sizes have been marked in the IGBP maps.

The GOME data is separated by IGBP class and snow cover, and file names are based on them: "GOME_LER_Bare_snow.dat" means bare land cover with some snow, and "GOME_LER_Bare_no_snow.dat" means bare land cover without snow. Each file contains the spectral LER values in all seasons for one land cover class. Data for all the wavelengths (335, 380, 416, 440, 463, 494, 555, 610, 670, 758, 772 nm) is presented, so that the data for the smallest wavelength (335 nm) is on the first row and for the largest (772 nm) on the last row (eleventh row). First column is LER in winter, second is the standard deviation for the winter measurements, third and fourth are for spring, fifth and sixth for summer and seventh and eighth for fall, thus each file has 11 rows and 8 columns. Wavelengths are not listed in the files.

The MODIS data is separated by seasons and snow cover, and file names are based on them: “MODIS_white_sky_albedo_winter_snow.dat” means winter measurements with snow, and “MODIS_white_sky_albedo_winter_no_snow.dat” means winter measurements without snow. Each file contains the spectral white-sky albedo values for all land cover classes both in northern and southern hemisphere in one season. Data for all wavelengths (0.47, 0.55, 0.69, 0.86, 1.24, 1.64, 2.13 μm) is presented, for more detail see RP-CAM-FMI-030.

The AVIRIS data is separated by land cover classes and file names are based on them: “AVIRIS_Grasslands.dat”. Each file has two columns: first is the wavelength in ascending order and the second one is the reflectance.

The ASTER data is separated by vegetation type or by land cover scenario, and file names are based on them: “ASTER_conifer_trees.dat” or “ASTER_urban_scenario.dat”. Each file has two columns: first is the wavelength in descending order and the second one is the reflectance.

The BRDF data is presented in one file: “POLDER_BRDF.dat”. There are 16 IGBP classes and 4 classes of NDVI with thresholds at 0.2, 0.5 and 0.8. For each of these 16x4 classes, we provide the BRDF parameters k1/k0 and k2/k0 at 6 wavelengths: 490, 565, 670, 765, 865, 1020 nm. The file has a header that explains the content of each column. The value 'ndvi' corresponds to the following intervals

0:	-0.2	< NDVI <0.2
1:	0.2	< NDVI <0.5
2:	0.5	< NDVI <0.8
3:	0.8	< NDVI <1.0

In addition to POLDER BRDF data we provide BRDF data from MODIS. These data sets are available at http://www-modis.bu.edu/brdf_albedo/gapfill5years_igbp.html. Pixels are filled with the mean values corresponding the IGBP Land Cover map. Pixels labelled as unclassified or deep water or permanent snow cover in the IGBP Land Cover map are filled with fill data. These maps are grouped within 20-degree latitude bands. No special tools are needed to read these data. There are only plain binary files, in BIP format with total 12 bands (representing 12 months). The data are 2-byte integers. All the files have been compressed into gzip format. P0, P1, and P2 in the file names are the three parameters of the MODIS BRDF model. P0 is for the isotropic kernel, P1 for the volumetric kernel, and P2 for the geometric kernel. B1 to B10 are the 10 MODIS land bands. For more details, please refer to the readme file at
http://www-modis.bu.edu/brdf_albedo/dat/v4/fill/Albedo/5yearsgapfill/readme.txt.

The ocean surface albedo spectra can be found in the COART_OCEAN folder. The file has two columns: first is the wavelength and the second is the albedo

2.8 Acknowledgements

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2.9 Appendix A. Parameter list of the data base.

name = parameter name, mlev = number of levels (1 = surface or integrated parameter, 19 = on all model levels), parameter = short description and unit.

```
name       mlev   Parameter
---------------------------
longitude    1   longitude [degrees]
latitude     1   latitude [degrees]
year         1   year
month        1   month
day          1   day
hour         1   hour [UTC]
aps          1   surface pressure [Pa]
phalf       20   half-level pressure [Pa]
pfull       19   full-level pressure [Pa]
zsurf        1   surface elevation [m]
t           19   temperature [K]
q           19   specific humidity [kg/kg]
rho         19   air density [kg/kg]
mass_air    19   total mass in layer [kg m-2]
xl          19   cloud water mixing ratio [kg/kg]
xi          19   cloud ice mixing ratio [kg/kg]
geopoth     19   geopotential height at full levels [m]
rhumidity   19   relative humidity [fraction]
tsurf        1   surface temperature [K]
albedo       1   surface albedo [fraction]
aclcac      19   cloud fraction
dms         19   DMS mass mixing ratio - gas phase [kg(S) kg-1]
so2         19   Sulfur dioxide mass mixing ratio - gas phase [kg(S) kg-1]
so4_gas     19   Sulfate mass mixing ratio - gas phase  [kg(S) kg-1]
so4_ns      19   Sulfate mass mixing ratio - aerosol mode nucleation soluble  [kg(S) kg-1]
so4_ks      19   Sulfate mass mixing ratio - aerosol mode aitken soluble  [kg(S) kg-1]
so4_as      19   Sulfate mass mixing ratio - aerosol mode accumulation soluble  [kg(S) kg-1]
so4_cs      19   Sulfate mass mixing ratio - aerosol mode coarse soluble  [kg(S) kg-1]
so4_tot     19   Total sulfate mass mixing ratio (aerosols) [kg(S) kg-1]
bc_ki       19   Black carbon mass mixing ratio - aerosol mode Aitken insoluble  [kg kg-1]
bc_ks       19   Black carbon mass mixing ratio - aerosol mode Aitken soluble  [kg kg-1]
bc_as       19   Black carbon mass mixing ratio - aerosol mode accumulation soluble  [kg kg-1
bc_cs       19   Black carbon mass mixing ratio - aerosol mode coarse soluble  [kg kg-1]
bc_tot      19   Total black carbon mass mixing ratio [kg kg-1]
oc_ki       19   Organic carbon mass mixing ratio - aerosol mode Aitken insoluble  [kg kg-1]
oc_ks       19   Organic carbon mass mixing ratio - aerosol mode Aitken soluble  [kg kg-1]
oc_as       19   Organic carbon mass mixing ratio - aerosol mode accumulation soluble  [kg kg-1]
oc_cs       19   Organic carbon mass mixing ratio - aerosol mode coarse soluble  [kg kg-1]
oc_tot      19   Total organic carbon mass mixing ratio [kg kg-1]
ss_as       19   Sea salt mass mixing ratio - aerosol mode accumulation soluble  [kg kg-1]
ss_cs       19   Sea salt mass mixing ratio - aerosol mode coarse soluble [kg kg-1]
ss_tot      19   Total sea salt mass mixing ratio [kg kg-1]
du_ai       19   Mineral dust mass mixing ratio - aerosol mode accumulation insoluble [kg kg-1]
du_as       19   Mineral dust mass mixing ratio - aerosol mode accumulation soluble [kg kg-1]
du_ci       19   Mineral dust mass mixing ratio - aerosol mode coarse insoluble [kg kg-1]
du_cs       19   Mineral dust mass mixing ratio - aerosol mode coarse soluble [kg kg-1]
du_tot      19   Total mineral dust mass mixing ratio [kg kg-1]
num_ns      19   Number mixing ratio - aerosol mode nucleation soluble [1 kg-1]
num_ki      19   Number mixing ratio - aerosol mode Aitken insoluble [1 kg-1]
num_ks      19   Number mixing ratio - aerosol mode Aitken soluble [1 kg-1]
num_ai      19   Number mixing ratio - aerosol mode accumulation insoluble [1 kg-1]
num_as      19   Number mixing ratio - aerosol mode accumulation soluble [1 kg-1]
num_ci      19   Number mixing ratio - aerosol mode coarse insoluble [1 kg-1]
num_cs      19   Number mixing ratio - aerosol mode coarse soluble [1 kg-1]
wat_ns      19   Aerosol water mass mixing ratio - aerosol mode nucleation soluble [kg kg-1]
wat_ks      19   Aerosol water mass mixing ratio - aerosol mode Aitken soluble [kg kg-1]
wat_as      19   Aerosol water mass mixing ratio - aerosol mode accumulation soluble [kg kg-1]
wat_cs      19   Aerosol water mass mixing ratio - aerosol mode coarse soluble [kg kg-1]
rwet_ns     19   Wet number median radius - aerosol mode nucleation soluble [m]
rwet_ks     19   Wet number median radius - aerosol mode Aitken soluble [m]
rwet_as     19   Wet number median radius - aerosol mode accumulation soluble [m]
rwet_cs     19   Wet number median radius - aerosol mode coarse soluble [m]
rwet_ki     19   Wet number median radius - aerosol mode Aitken insoluble [m]
rwet_ai     19   Wet number median radius - aerosol mode accumulation insoluble [m]
rwet_ci     19   Wet number median radius - aerosol mode coarse insoluble [m]
tau_2d       1   Total column aerosol optical depth at 550 nm [unitless]
m_tot_dry   19   Total dry aerosol mass mixing ratio [kg kg-1]
m_tot_wet   19   Total wet aerosol mass mixing ratio [kg kg-1]
pm_25        1   Dry mass of aerosols with diameter < 2.5 Âµm, lowest layer [kg m-3]
pm_100       1   Dry mass of aerosols with diameter < 10 Âµm,  lowest layer [kg m-3]
f_fine_dry  19   Fraction of dry mass in particles with dry diameter < 2.5 Âµm [unitless]
f_fine_wet  19   Fraction of wet mass in particles with wet diameter < 2.5 Âµm [unitless]
```

3 Complementary Observations and Delivery Requirements

3.1 Introduction

This Task within the Camelot study assessed two aspects: firstly, the auxiliary data requirements associated with operational systems and hence required for the mission concepts for air quality and climate monitoring; secondly, the near-real time requirements for air quality applications.

The range of applications examined in this report, and their maturity, are constantly in a process of evolution, and therefore this report can provide only a snapshot of current capabilities and expectations; indeed the user base is growing as interface systems to satellite data become more advanced and different techniques are employed for different applications. Nonetheless there is a maturing methodology in the area of air quality and climate monitoring at least as regards the outputs of this Task i.e. auxiliary data and speed of delivery.

To re-iterate, the focus of the Camelot study is to address the definition of air quality and climate protocol monitoring missions, the so-called B1, B2 and C1 user requirements in the Mission Requirements Document (MRD).

The area of auxiliary data is quite extensive for these missions, as for any atmosphere mission addressing a range of trace gases. We can distinguish auxiliary requirements ranging from necessary algorithm inputs to quality control and assurance (QC/QA) to auxiliary data required for end user applications such as the EC core services.

Three areas are covered in this operational report:

1. Auxiliary data required as **inputs for data processing systems** such as data retrievals (algorithms producing Level 2 and Level 3 products).
2. Auxiliary data required for **quality control and quality assurance** of operational products (validation for operational systems).
3. Auxiliary data required for key, higher level, **application area**s in the core and downstream services, including data assimilation systems (Level 4 products).

These aspects have quite different impacts and require separate treatments although in some cases, such as meteorology, a commonality across all areas may be identifiable. In addition, in area 3 one has to maintain a reasonable dialogue with application experts so that the correct sharing/updating of information can occur.

Auxiliary inputs for **data processing systems** essentially consist of variables not measured, which must be specified either by climatology or by auxiliary inputs e.g. meteorological analyses and surface variables. In addition, variables can be identified which need to be measured, including aerosols and clouds; water vapour is another common requirement for all applications. The analyses presented here are based on questionnaires, literature surveys and the analyses of Task 3.

Auxiliary inputs for **quality control/quality assurance systems** essentially consist of validation systems for which similar methods were used to assess performances: the CAPACITY report, questionnaires, literature surveys and Task 3 outputs. An emphasis has been placed on current operational and pre-operational systems such as EMEP, national air quality monitoring systems, NDAC, AERONET and other similar networks. The CAPACITY report noted that (institutional) users would prefer validated data sets with well-established uncertainties in terms of accuracy and possible biases. This requires both validation of observations and, most importantly, assimilation models, a subject that is considered briefly below.

For higher-level products including data assimilation, a key delimiter is the extent to which such activities occur in the ESA/EUMETSAT ground segment area or in the EC core and downstream services. In this report, it is assumed that it is in fact the EC atmosphere service, a successor to GEMS and PROMOTE, which will incorporate the assimilation effort. Therefore in this report, we concentrate on identification of primary auxiliary variables, which require satellite observations directly as part of an atmosphere mission, rather than on secondary auxiliary inputs (for example emission databases) that will be needed as part of core or downstream services.

Even with these restrictions, it is worth noting that there are auxiliary data sets which will support the **application areas**. This list is not comprehensive but does reflect some of the key inputs from other Sentinels that will be of value, particularly Sentinel-3.

3.2 Auxiliary data for retrievals

The expected systems for air quality and climate monitoring currently aim to target a number of species, some of which are in common. For air quality, O_3, NO_2, CO, SO_2, CH_2O, aerosol optical depth (OD), aerosol types, HNO_3, PAN, N_2O_5 (night) and spectral UV surface albedo comprise the targets for protocol monitoring and near real-time air quality. For climate, CH4, CO, CO_2, O_3, NO_2, aerosol OD (total and absorption) are required for protocol monitoring.

Auxiliary data for retrievals comes in a number of different forms. One can identify three sub-sets of data, each with sub-categories and each with a starting point that is defined.

1. Auxiliary databases - “Pre-defined” sets of data
   - Atmosphere Climatologies: e.g. a priori data and interfering gases/aerosols
   - Surface parameters: e.g. albedos, emissivities, fractional vegetation
   - Process variables for *application areas*: e.g.

2. Input data sets: coincident satellite datasets and analyses
   - Metop/NPOESS/… observations, e.g. water vapour, cloud cover
   - MSG/MTG Observations, e.g. cloud cover
   - Met analyses e.g. ECMWF temperature, pressure, humidity.

3. Expanded measurements: additional retrievals
   - Simultaneous retrievals
   - Additional channels

As a result of the study, two sets of tables have been compiled, one showing which auxiliary data are required (Table 3-1 and Table 3-2) and the second showing indicative quantitative estimates for the accuracy requirements currently for these parameters (Table 3-3 and Table 3-4). These tables have been further sub-divided into broadband spectral influences, i.e. clouds, aerosols and surfaces (Table 3-1 and Table 3-3), and the second showing indicative quantitative estimates for the accuracy requirements currently for these parameters (Table 3-2 and Table 3-4 respectively). Information on the tables is supplemented with information from published papers which are referenced where possible.

The table columns are ordered in terms of wavelength from ultra-violet (UV), through near infrared (NIR) and shortwave infrared (SWIR) to thermal infrared (TIR). Note that all retrievals have a requirement for cloud knowledge but in some cases, such as the TIR, this is currently only to provide a threshold for cloud flagging and use of data for inversion in the retrieval scheme.

In Table 3-1 and Table 3-2, an *X* indicates that the auxiliary variable is required. Where it does not but the box contains a (coloured) symbol, then there is an influence of that variable on the radiative transfer but its measurement requirement is not clear from the literature. In some cases, inclusion of the interfering auxiliary variable as a retrieval variable will be sufficient to mitigate its influence on the retrieved concentrations but in others this reinforces the need for particular supplementary channels.

The key aspects required for retrievals which can meet the MRD user requirements are cloud flagging/cloud top pressure, aerosol knowledge, temperature/pressure and water vapour. In the wavelengths for which scattering in the atmosphere occurs rapidly (UV through to SWIR), knowledge of the photon path is very important for the highest accuracy and this leads to a requirement for the co-measurement of a relatively well-mixed gas such as O_2, O_4, or CO_2 (see also section 5 and Task 3 report). The O_2 A-band measurement potentially provides the most accuracy if observed with sufficient resolution but is somewhat separated in wavelength from the SWIR measurements for which CO_2 has commonly been used for CH_4 and CO.

Table 3-1. List of spectrally broadband auxiliary variables required for retrievals (aerosol, cloud, surface); X= Required; L= Large aerosol particles; D = dust; A = Albedo; E= emissivity; IRC = Infrared clouds; SC=SWIR Clouds.

TARGET GAS	**O_3**	**SO_2**	**NO_2**	**CH_2O**	**H_2O**	**CO**	**CH_4**	**CO_2**	**CO**	**O_3**	**HNO_3**
Spectral range	UV	UV	VIS	VIS	NIR	SWIR	SWIR	SWIR	MIR	MIR	MIR
Cloud Fraction	X	X	X	X	X	X	X	X	IRC	IRC	IRC
Cloud CTH	X	X	X	X	X	SC	SC	SC	IRC	IRC	IRC
Cloud albedo	X	X	X	X	X	SC	SC	SC			
Aerosol ext	X	X	X	X	X	X	X	X	L	L	L
Aerosol type	X	X	X	X	X	X	X	X	D	D	D
Surface elevation	X	X	X	X	X	X	X	X	X	X	X
Surface pressure	X	X	X	X	X	X	X	X	X	X	X
Light path +column (O2, O4, CO2)	X	X	X	X	X	X	X	X			
Albedo/emiss	XA	XA	XA	XA	XA	XA	XA	XA	XE	XE	XE

Table 3-2. List of trace gas auxiliary variables required for retrievals including data from satellite instruments (SAT), analysis fields (Analy), chemical transport models (CTM) and climatology; T= Target gas, C=Current, F=Future (expected), P/V = Polluted/Volcanic

GAS	**O_3**	**NO_2**	**SO_2**	**CH_2O**	**CO**	**CH_4**	**CO_2**	**H_2O**	**CO**	**O_3**	**HNO_3**
Spectral range	UV	VIS	UV	VIS	SWIR	SWIR	SWIR	NIR	MIR	MIR	MIR
Analy P/T	C	C	C	C	C	C	C	C	C	C	C
Analy H2O					C	C	C		C	C	C
SAT P/T					F	F	F		F	F	F
SAT H2O					F	F	F		F	F	F
PROFILES	X	X	P/V	X	X	X	X	X	X	X	X
CTM	X	X		X			X (OCO mission)				
Climatology	T	T	T	T	T	T (CO_2)	T	T	T	T	T

The strong conclusion is that very good knowledge of clouds and aerosols is required to meet user requirements. These necessitate use of the O_2 A-band for both air quality and climate monitoring in the UV-visible and NIR/SWIR bands. The use of O_2 A-band is recognised in the MRD and its use is demonstrated in Task 3.

A second strong conclusion is the measurement requirements are best met by also including well-mixed gases observed at closely related wavelengths to the target gas. In particular, current state-of-the-art retrievals for CH_4 use the CO_2 proxy method, based on the proximity near 1.6 µm of both CH_4 and CO_2 bands. Therefore the system for monitoring CH_4 should include a 1.6 µm channel with the ability to measure CO_2. This option is studied further in Task 3.

A related element to the photon path normalisation is the use of surface pressure/vertical density variations for conversion of total column measurements to mean dry mole fractions or mixing ratios (see section 5). The OCO approach is to retrieve surface pressure as one of the parameters. Aerosol and surface pressure considerations have been tested in Task 3 utilising the O_2 A-band.

Two auxiliary data sets that are now increasingly required for retrieval algorithms are the following: 1) surface albedo/emissivity; 2) digital elevation models. The requirements for surface albedo and digital elevation are better established in the UV, visible, NIR and SWIR ranges than in the thermal infrared; surface albedo in the SWIR may not be well-known. Retrieval studies in Task 3 indicate that retrieval schemes show less sensitivity in the thermal infra-red to surface emissivity, mainly because of decreased sensitivity near the surface compared to reflected sunlight measurements but also because of the lower sensitivity to aerosols allowing better discrimination of the surface radiation term.

Mean surface elevation is typically required to better than 100 m within the trace gas pixel for measurements, which use scattered sunlight. Thermal infrared measurements are less sensitive but are likely to require maps of mountainous terrain. The ground segment is likely to need to utilise an external source of digital elevation model, high accuracy versions of which are being developed as part of other ESA satellite systems.

Input profile data for temperature and pressure comes from either the infra-red sounder or the Meteorological forecast/analysis satellite system; it is likely that the forecast and analysis systems have assimilated satellite data over the ocean but not over land. Performance of the Infrared Atmospheric Sounding Interferometer (IASI) data indicates that thermal infrared profiles of temperature are good to 1 K except close to the surface (2 K). Errors in water vapour retrievals are closer to 10% for IASI and have been investigated further in Task 3.

A very important development is the use of model data for two very important steps: 1) to calculate the stratospheric columns using a stratospheric CTM, e.g. for NO_2; 2) to use global tropospheric chemical transport models, e.g. for CO_2 as might be done for OCO, or regional models, such as EURAD for NO_2, to provide vertical profile shape information. Then, as trialled in the PROMOTE service the tropospheric slant column density is obtained by subtracting the stratospheric column slant density from the total slant column density. The tropospheric column is then derived using air mass factors calculated using the tropospheric profile shapes using meteorological data to compute partial columns.

Hence a key issue for the ground segment is the type of data to be delivered and the processing to be performed. Whichever route is chosen, total slant column data should be provided so that users can perform their own stratospheric/tropospheric corrections, for example in the core services.

Table 3-3. List of spectrally broadband auxiliary variables for retrievals and estimates on their knowledge.

GAS	O_3	NO_2	SO_2	CH_2O	H_2O	CO	CH_4	CO_2	CO	O_3	HNO_3
Spectral range	UV	VIS	UV	VIS	NIR	SWIR	SWIR	SWIR	MIR	MIR	MIR
Cloud Fraction		20% (1		20% <40 %	< 50%	20%	0% SCIA (some algorithms – 100% cloud-free)	0% SCIA (some algorithms); OCO – 0.3 optical depth			0% (cloud-fee only)
Cloud CTH/pressure	100 mb	1-2 km		1-2 km							
Cloud albedo		0.2		0.2			0.01	0.01			
Aerosol ext	20 % aerosol optical depth					5 – 20 % aerosol scattering		<0.05 optical depth			
Aerosol type											
Surface elevation	50 m	100 m		100 m		100m	10 m	50-100 m			
Surface pressure							2 mb	1 mb			
Albedo/emissivity	A 0.02 Snow/Ice 0.05	A 20%		A 20%			A < 5%	A < 5-10%	E 20 %	U	U

1) Relative error for cloud fractions of the order 0-0.2.

Table 3-4. List of trace gas auxiliary variables for retrievals and estimates on their knowledge.

GAS	O_3	NO_2	SO_2	CH_2O	H2O	CO	CH_4	CO_2	CO	O_3	HNO_3
Spectral range	UV	VIS	UV	VIS	NIR	SWIR	SWIR	SWIR	MIR	MIR	MIR
Analy P/T	1 - 2K required	10%				2 K assumed	1 K	Depends on algorithm?	1-2 K	1-2 K	1-2 K
Analy H2O								Depends on algorithm	10%	10%	10%
SAT P/T									1-2 K	1-2 K	1-2 K
SAT H2O									10%	10%	10%
PROFILES	X	X	X	X	X	X	X	X	X	X	X
CTM	X	X		X							
Climatology		20 %		< 30 %				< 10%			
Spectral cross-sections	1 % required	<5% precision, <10% accuracy			< 5% precision	<25%	< 2%	< 1%			

3.2.1 Summary

For all the parameters noted here as being important, the estimates of sensitivity are derived from the literature and the simulations in Task 3 and 4.

The strong conclusion is that very good knowledge of clouds and aerosols is required to meet user requirements. These necessitate use of the O2 A-band for both air quality and climate monitoring in the UV-visible and NIR/SWIR bands. The use of O2 A-band is recognised in the MRD and its use is demonstrated in Task 3. For clouds, one can identify cloud fraction, cloud top height/pressure and cloud optical depth; for thermal infrared measurements, cloud top temperature is also required but can possibly be inferred from cloud top height/pressure.

The O2 A-band is also important for providing a measure of surface pressure although this study did not address whether surface pressure errors are lower from the satellite retrievals than the accuracy achievable in meteorological systems.

A second important conclusion at this stage is the requirement for measurement of the scattering light path directly via O_2, O_4 or CO_2. This is now standard for many measurements. For SWIR measurements (CH_4 and CO), CO_2 represents the appropriate variable because of the closeness of wavelengths albeit with a larger mixing ratio variation than for O_2. The required output product is now, for example, XCH_4 and XCO2.

Aerosol extinction and aerosol type data are required, as was already known. There needs to be a discrimination between large (coarse) and small (fine) particles. Aerosol measurements were studied in Task 3. For the thermal infrared instruments, large dust particles must be measured at night; thermal infrared aerosol measurements should be assessed in the future. The areas where these will have an influence are well-known.

Input profile data for temperature, pressure and water vapour data come from either the infra-red sounder or the Meteorological forecast/analysis satellite system; it is likely that the forecast and analysis systems have assimilated satellite data over the ocean but not over land. It is assumed that the performances similar to those of the Infrared Atmospheric Sounding Interferometer (IASI) data will be achieved and this is sufficient for auxiliary data requirements.

Surface albedo/emissivity sensitivities are known to exist and databases for the ground segment will be required.

Surface elevation should be well known and digital elevation models will be required for the ground segment.

For user accessibility, a number of products should be provided as outputs of the ground segment: slant columns, total columns, stratospheric columns and tropospheric columns. A number of core users will utilise Level 1 spectral radiance data directly also and these should also be provided

The utility of model data within the retrieval processor needs to be considered e.g. for the shapes of tropospheric profiles and knowledge of the stratospheric burdens of some species. This implies that measurements of stratospheric concentrations of NO_2 and O_3 are important.

3.3 Auxiliary data for validation QC/QA

All of the target measurements for the air quality and climate monitoring missions require validation both for quality control and quality assurance. In both respects, for operational purposes, what is required are long-term, quasi-continuous measuring systems providing standard data sets to a cal/val environment associated with the ground segment. The large the number of coincidences with validating instruments, the greater the significance that can be attached to any output product from the satellite system. In addition, an updatable data quality summary can then be provided which is essential information to be output for core service and downstream services. Although it is not the primary function of this report or this section, it is important to note that both the validation environment and user services will require atmospheric products with characterization data (such as cloud flags and averaging kernels) and appropriate error estimates, suitable for user implementation.

For QA/QC work, one can distinguish sub-sets of the data in the following manner, with identified starting points:

1. Validation datasets
   - Data sets are required to validate each output parameter to at least the same accuracy/precision.
   - Ground-based remote sensing systems
   - Ground in situ
   - Airborne systems: aircraft and balloon
   - Process variables from met. analyses or geophysical correlations.

   Starting point: ENVISAT/Aura validation studies, CAPACITY studies, EU Geomon study (this study has just started)

2. QA

   Quantities that may be used to flag data quality
   - Cloud observations
   - Surface conditions
   - Humidity
   - Aerosol

   Starting point: ENVISAT/Metop validation, Task 5 results (clouds).

Of the validation techniques, one can divide these into long-term, statistically based validation data sets and specific campaign deployments. Long-term data sets consist of ground-based remote sensing systems and ground in-situ systems; however these long-term data sets will need to be certified by inter-comparison, inter-calibration and also testing for atmospheric conditions. Aircraft and balloon validations are more likely to occur as sporadic campaigns or regular flights but with large time gaps between deployments. There are also geophysical QA/QC procedures that can also be implemented for QA/QC, e.g. variability of products in areas of low geophysical variation, dependence on albedo or solar zenith angle.

An important issue is that the error statistics for a given product will depend on cloud content, surface conditions, humidity and aerosol to name the largest common influences on target product accuracy. Therefore the output data quality should in principle also provide information on the coincident data for these auxiliary variables or at least provide a quality flag based on these data outputs.

The results of this study have been collated in Table 3-5 from questionnaires together with literature searches and the survey of ground-based instruments performed in the CAPACITY study. The MRD requirements in Table 3-5 are synthesized from the current MRD (sentinel 4 and 5 MRD issue 1 rev 0.pdf) and form a convenient summary. Essentially the assumption in using the CAPACITY assessment is that the validation instruments should achieve at least the accuracy requirements of the target MRD requirements, in which case one can use the assessment of current ground-based systems in the CAPACITY report to infer successful validation.

A further issue is that although all the requirements are met in principle for gases, such as for example NO_2, nonetheless it is clear that knowledge of horizontal variability is important. Although it has been show that these factors can be taken into account, ties to the in situ network require further research to be conducted to provide full performance. Urban validation of NO_2 is a particular concern but also for gases with high tropospheric variability. It is also clear that it is important to have a good knowledge of the validation site factors such as stratospheric concentrations and surface albedo. Some of the best validation sites may therefore consist of in situ and remote sensing instruments in coincident locations. In addition, many coincidences are needed to give the comparisons statistical significance.

Table 3-5. Comparison of target gas requirements and performances of validation sensors.

Species	MRD REQS MAX	MRD REQS MIN	SYSTEM	ASSESSMENT BASED ON CAPACITY	CURRENT ESTIMATES	LIKELY FUTURE PROGRESS	UNCERTAINTY	MEASUREMENT TYPE
CH_4	2% (TRC)	2% (TOTC)	IN SITU (PBL) FTIR	Requirements not met although CAPACITY would conclude they are met	2-7% for FTIR	0.5% may be needed	<5% precision 7 % accuracy	Ground based FTIR (total column)
CO	20% (PBL)	25% (TOTC)	IN SITU (PBL) FTIR	Requirements met	7 % for FTIR	More stations required	<5% precision 7 % accuracy	Ground based FTIR (total column)
							2 – 3 % precision	NSDC = Ground based FTIR
							5% precision	GAW = in situ surface sampling sites
CO_2	0.5% (TRC)	0.5% (TOTC)	FTIR	Requirement not met	<0.3 ppm (precision) <0.1 ppm (accuracy) which would meet requirements	TCCON FTIR network (OCO)	~0.1 % precision ~0.3% accuracy	FTS (as part of the TCCON)
			[IN SITU for PBL]	[2%]			<5% precision 3% accuracy	Ground based FTIR (total column)
NO_2	10% (PBL)	1.3e15 molec cm^{-2} (TOTC)	IN SITU (PBL) UVV-MAXDOAS, UVV DOAS, SAOZ (FTIR)	Requirements can be met but only by DOAS instruments and problems in urban areas. Needs network of stations determining key inputs and outputs of satellite NO_2 system	5-20%		200 pptv precision 8% accuracy	DOAS
							2 to 5% precision < 5% accuracy	In situ: PCL = Photolysis to NO followed by chemiluminescence LIF = Laser induced fluorescence
							< 50% Total error (worst case scenario for total column)	In situ (PBL)
O_3 COL	3% (TOTC)	25% (TRC)	MAX-DOAS, UVV DOAS, FTIR, Dobson	Requirements met			1-3 % accuracy	Dobson
							5% accuracy 2% precision	SHADOZ ozone sondes (total column)
O_3 PROF	10% (PBL)	20% (FT)	IN SITU + SONDES (NDACC/SHADOZ) meet PBL reqs. SONDES AND FTIR MEET FT	Requirements met	5% for SONDES.		2% precision 5% accuracy	NDSC ozone sondes
							5- 10 % precision < 3 % systematic	ECC sondes
							10-20% precision < 5% accuracy	Non- ECC sondes

Species	MRD REQS MAX	MRD REQS MIN	SYSTEM	ASSESSMENT BASED ON CAPACITY	CURRENT ESTIMATES	LIKELY FUTURE PROGRESS	UNCERTAINTY	MEASUREMENT TYPE
SO_2	20% (PBL)	1.3e15 molec cm^{-2} (TOTC)	IN SITU (PBL) UVV MAXDOAS	Requirements are met			0.33 % precision	UV-DOAS
CH_2O	20% (PBL)	1.3e15 molec cm^{-2} (TOTC)	IN SITU (PBL)? UVV MAXDOAS	Requirements are met (PBL check)	20%	SAME BUT 10%	0.37 % precision	UV - DOAS
							~ 5% accuracy ~9 % precision	MAX-DOAS Po-VAlley
							< 6 % total < 3 % Systematic	DOAS White system
H_2O	10% (PBL)	10% (TOTC)	IN SITU	Requirements partially met (PBL but not TOTC)				
PAN	20% (PBL)	1.3e15 molec cm^{-2} (TOTC)	IN SITU	No assessment				
HNO_3	20% (PBL)	1.3e15 molec cm^{-2} (TOTC)	IN SITU (PBL) FTIR	Requirements are met			11 – 14 % accuracy 3.2 – 8.5 % random	FTIR (Arrival heights solar and lunar measurements)
N_2O_5	20% (PBL)	1.3e15 molec cm^{-2} (TOTC)	IN SITU	No assessment				

3.3.1 Summary

Overall, the validation auxiliary data looks to be in good shape, but some key issues must be addressed and data will need to be gathered and utilised in an efficient manner. Collection of data and operability are issues that will need to be considered.

The key issues are the accuracy of greenhouse gas measurements achieved by the FTS systems in the NDACC and TCCON networks, the spatial representivity and accuracy of MAX-DOAS systems, and the ties between the remote sensing instruments and the surface in situ network (particularly for air quality). For air quality, urban validation is a significant issue. Excellent progress has been made in recent years and could enable the requisite performance to be achieved by the time of flight of the Sentinels.

The nature of the validation information is likely to be important and at least for some sites knowledge of local site conditions, trace gas variability and stratospheric burdens will be required. Good numbers of coincidences are required for statistical significance to be associated with the comparisons.

For NO_2, a key measurement target, there is a key requirement for an independent operational network of sensors delivering information that can verify both the inputs to the satellite processing system and the outputs of that system. This network needs to cover both urban and rural sites, including rural outflow and with investigation of NO_2 lifetimes. In addition to continuous measurements of both total and tropospheric columns, there is also a need to deliver good information on the stratospheric NO_2 column, the tropospheric NO_2 profile, the NO_2 diurnal cycle and the presence of aerosols and clouds.

These considerations are increasingly being understood and activities are being undertaken within ESA and the EC Geomon project to begin to address these issues. However, a particular need is to move from campaigns-only mode to emphasise also a network of operational in situ sensors. A network is the only to achieve both the required long-term accuracy and local characterisation, but also to ensure good statistics, seasonal and weekly cycle coverage, and true assessment of trace gas variability. Such a system could also include in situ sensors but their placement and accuracy, e.g. with respect to conversion efficiency, would need to be carefully assessed.

3.4 Auxiliary variables for air quality

The intended foci for the missions considered in the CAMELOT study can be broken down into air quality and climate. In this section, we examine air quality.

The air quality area is complicated as 1) there are a number of ways in which satellite data can be used in the air quality problem; 2) there exist a large range of air quality models with different domain applications, formulations and target regions and accuracies. Therefore, a survey of the chief areas was performed as well as direct contact to users.

Satellite data could be used in air quality in a number of different ways:

- Spatial and temporal footprints of pollution
- Regional modelling and air quality forecasting
- Inverse modelling of emissions
- Protocol compliance monitoring
- Long-range transport of pollutants
- Long-term trends in pollutants

These are now considered in turn.

3.4.1 Spatial and temporal footprints of pollution

One of the expected advantages of satellite data are the opportunities to examine a broader spatial and temporal view of the extent of pollution with coverage of regions not directly sampled by in situ networks. In addition, the satellite data might provide a better view of mean conditions as opposed to the site dependent characteristics of the sparse network of sensors currently deployed with a bias towards large urban conurbations rather than smaller settlements and rural areas.

Studies such as Beirle et al. [2003], Kramer et al. [2008] and Blond et al [2007] have already examined the spatial patterns of NO_2 and the daily loading of the atmosphere that occurs as a function of time on global, regional and city-scales.

As for the previous application, there is no obvious requirement for auxiliary data directly from satellite as part of the initial application of the data. Assessment and regulatory agencies, as well as modellers, would prefer to be able to examine this spatial variation in the context of meteorology and land cover (urban/rural domains). In addition, road traffic and road mapping databases would also be utilized. In some areas, e.g. the Southern Mediterranean, the influence of local fires/biomass burning would be important information. These aspects are in common with those discussed in the next section and are better covered there.

For this application, the auxiliary data aspects are elements, which would be expected to be provided by core and downstream services rather than coincident measurements from the atmosphere sentinels. Nonetheless, it is important to note the use of Sentinel 1-3 data for land cover and the provision of such high-resolution data to the atmosphere services for air quality. Meteorological data will most likely be acquired directly by service centres although it may be best to supply the meteorological data directly from the atmosphere ground segment to allow users to use consistent data sets. These data may, in future, also be used to drive local mesoscale meteorological models.

3.4.2 Regional modelling and local/regional air quality forecasting (including long-range transport of pollutants)

This is a complex area with a mixture of commercial and public institute models. Local air quality models do not currently make use of satellite data although a number of large and small cities such as Madrid, Leicester, and London are either making use of satellite data indirectly or are interested in doing so. In the most case, these local models do not directly assimilate the in situ data, except perhaps in France, but use these data for scaling either in an automatic or manual (duty forecaster) manner.

Satellite data may be used in two ways. The first is as an average scaling load, analogous to the use of in situ data, for which the satellite data has some advantages since it represents a mean concentration on the satellite grid scale. The utility of this use of satellite data has been demonstrated by comparison to in situ data in the Po Valley and Leicester (Kramer et al. [2008]) where knowledge of the horizontal spatial heterogeneity of the scene in NO2 provides for a better result. Blond et al [2007] have also shown that satellite data and CHIMERE model data are well correlated, except in winter, and that the satellite data can provide correct factors for the model. The second is through the assimilation of satellite data into a regional model. This is the standard route for application of satellite data where the model/satellite data can provide the local model with knowledge of the background and transported fields. The PROMOTE and GEMS projects have been working on these methods and it is expected that the new EC thematic centres will implement these assimilation approaches. In effect the satellite data contributes at the moment to the initial value knowledge rather than emission rate knowledge although inversion to both would be desirable [Elbern and Strunke, 2005].

For both these applications, it should be recalled that many air quality models are very local and do not have good specification of requirements. Rather it is the case that satellite data will improve the air quality system as a matter of course providing additional information that was not available before.

For the first application, the direct application of the satellite data requires no auxiliary data at the satellite end; the user will have requirements for emission inventories, first order model calculations of the high spatial resolution field, and meteorology but these are separate and location-dependent. Therefore there are no auxiliary data requirements.

For the second application, assimilation into a model, discussions were held with expert users at AEA Technology (with CERC experience) and the University of Cologne. There is a large area where services such as PROMOTE and GEMS are already involved using the regional models. The integrated air quality service of PROMOTE currently expects to employ the EURAD, CHIMERE, MOCAGE, LOTOS-EUROPE and SILAM models. The GEMS service has proposed to test MOCAGE, BOLCHEM, EURAD, CHIMERE, SILAM, MATCH, CAC, MM5-UAMV, EMEP, REMO, and UMAQ-UKCA.

The following variables are suggested to be important:

Fast data (near real-time)
Meteorological data for winds (direction, speed), temperature (and humidity).
Convective skill as models become more sophisticated and higher spatial resolution.
Local in situ network data

Databases or parameterisations
Land use, e.g. CORINE. These databases are typically currently static but should be dynamic.
Emission inventories which are either internal or delivered from EMEP or are local to a city application.
Soil Moisture.

Transport influences
Regional and global target gas distributions.
Meteorological data is required again.
Data on biomass burning, e.g. EO data for fires, tracers such as CO and aerosols.
Transport of dust and volcanic aerosols (also SO_2).

Chemistry influences
Photolysis rates, particularly of NO_2 (with requirements for cloud, cloud optical depth, aerosol optical depth and weakly for overhead O_3 which is mainly stratospheric).
Volatile organic compounds (particularly in VOC-limited regimes)

Unknowns
Atmospheric mixing height, atmospheric stability (in effect boundary layer height).

Currently the auxiliary data not covered are the fire data which is clearly of utility and the CORINE land cover data but the latter should be available through the EC land core service. Good data on dust and volcanic aerosol are desirable, i.e. aerosol type information, and have been studied in Task 3. Data on hydrocarbons and biogenic volatile organic compounds would be useful although it is not yet clear that these can be measured from space in the lower troposphere, aside from formaldehyde and glyoxal. Finally, temperature is a driver of surface emissions and chemistry suggesting that surface temperature and air temperature are both important.

Finally the use of imagery, of the MODIS form, for assessing transport of aerosols particularly from fires came across clearly in our investigations. It is clear that easy access to repositories of images is of utility for both near real-time and post-event analysis of pollution events. Complementing access to image data would be the availability of fire data. Since events may occur at some distance and time from the application area, it is not necessary to have a fire monitor directly on the air quality satellite, although it would potentially be useful.

3.4.3 Inverse modelling of emissions

Inverse modelling studies of emissions, for example from NO_2, are beginning to reveal some interesting information for regional emissions analysed on a global basis and also on a detailed “scale of city” basis in Western Europe. It has been shown satellite data may be used to verify the emission inventories employed in regional chemical models and to estimate their uncertainties. On a global basis, additional sources of EO data are particularly fires, global burned area, and aerosol data (aerosols are a target) although sources of nitrogen oxides such as lightning may also benefit from relevant EO data.

3.4.4 Protocol Compliance Monitoring

Protocol compliance monitoring is continuing to be assessed as a utility of satellite data. Aside from sampling issues, there are also issues of data quality, validation and bias assessment. However, there are no direct requirements for auxiliary variable information for interpretation of the target product data, such as NO_2, except that which might be required for the error and quality flagging of the data as discussed previously. Hence at this time there are no expectations of auxiliary data to be required for protocol compliance monitoring.

3.4.5 Long-term trends in pollutants

Satellite data for pollutants form the best method of monitoring long-term trends in pollutants, over much of the globe and particularly in remote regions. Richter et al. [2005] showed the development of NO_2 over China and the increasing influence there. As for protocol monitoring above, there is no expectation a priori that additional EO data sets are needed although for more difficult cases, data quality will have to be shown to be robust. In addition, there may be variables that aid in the interpretation of trends. Nonetheless at this stage, a reasonable conclusion is that there are no auxiliary variables that are required at this stage.

3.4.6 Summary

The investigations performed in this study have found an increasing body of work in the area of air quality and utilization of satellite data with some encouraging results. Air quality models range in forms from complex regional chemical-transport models to detailed local meteorologically driven models to simpler local scaling versions. Therefore their sensitivities to key parameters and their requirements for auxiliary data differ considerably. Nonetheless, two things are clear. Firstly target air quality satellite products and auxiliary data will be of use in improving air quality forecasts and knowledge. Secondly, the auxiliary data of use is mostly of the same form for utilization and for interpretation.

For the target products, in addition to the current suite it was found to be desirable that a satellite product estimating the photolysis rates for NO_2 should be produced, based on the user survey and published literature. For the photolysis product, it would be very useful to have as inputs good aerosol and cloud optical depth data which are data sets therefore offering extra capabilities to the air quality model. These data sets can be produced by the Sentinel 4/5 system and good information is also available, in principle, from Sentinel-3.

Easily accessible daily image data of the MODIS form are highly desirable and appear in user reports on air quality. Sentinel-3 OCLI and SLSTR could satisfy these requirements for the future and this use for atmosphere applications should be supported.

For auxiliary data, it was found that the most desirable aspects were aerosol with dust separation, fires, land cover, and temperature. Meteorological data are a necessity. It is assumed here that these are available through the EUMETSAT and meteorological organizations.

3.5 Auxiliary variables for climate

Satellite data could be used in climate in a number of different ways:

- Protocol compliance monitoring
- Spatial footprints of emissions
- Assimilation and global/regional modelling of climate gases
- Inverse modelling of global and regional emissions
- Long-term trends in climate gases

Discussions were held with experts from the ECMWF and the LSCE-CNRS.

For the climate area and for greenhouse gases in particular, the situation is rather simple compared to air quality. The chief uses of the data currently are in inverse modelling for emissions, assimilation and long-term monitoring, all of which impact on protocols.

3.5.1 Inverse modelling of emissions

In inverse modelling, the requirements are clear. For the target species themselves, the use of mean dry mole fraction or mean dry air mixing ratio is standard – the product is often denoted as XGas so XCO_2 or XCH_4. Therefore, the column data need to be transformed, a process which occurs either through use of the normalisation to CO_2 and O2 columns (thus also reducing photon path errors) or through the use of surface pressure (see also Section 2).

For auxiliary data for greenhouse gas inverse modelling, the most important parameters are fire (burned area), land cover maps, vegetation intensity indication (e.g. FaPAR, Leaf Area Index) for land; ocean colour and sea surface temperature for the ocean; atmospheric chemistry observations which constrain OH. For the CO_2, CH_4 system, OH will be constrained by CO although methyl chloroform is more standard. Note that CO measurements are required for CH_4 inverse modelling since CH_4 and CO are inter-linked.

For other climate components, inverse modelling of NO_2 falls under the air quality discussion above whilst inverse modelling of aerosols is in its infancy. However precursor gas concentrations, such as SO_2, would be useful as would measurements of photolysis rate (as discussed in section 4).

3.5.2 Data assimilation for climate

In terms of data assimilation, systems such as the GEMS system, and follow-on European core services, currently assimilate O_3, NO_2, CO, AOD, CO_2 and CH_4 (both trace gas data and radiances). For gases such as CO_2, CH_4 and CO, the issues are similar to those discussed under inverse modelling. However, the assimilation would benefit also from up-to-date flux climatologies, sometimes blended with a model; this is likely to be an output from a core service rather than the satellite ground segment but shows the requirements for averaged data as well as individual measurements. The most difficult observation to constrain is aerosol a more diverse aerosol set, including type, is required.

The meteorological systems are the foundation of assimilation schemes and are moving towards better representations of clouds, for example. It is beyond the scope of this study to improve the meteorological system beyond that intended for MSG/MTG and Metop/post-EPS. There is an issue with measurements of clouds and cloud optical depth which would improve the climate and air quality applications, particularly for convective clouds.

It is worth noting that in-situ data are of high importance for the proper assimilation of satellite data. In-situ data are needed to anchor the assimilation system in terms of biases as well as being used for validation and quality control.

It is likely that the assimilation models under core or downstream services will want to assimilate radiances directly at all wavelengths. Hence Level 1 calibrated spectral radiance data will need to be an output product of the ground segment.

3.5.3 Long-term monitoring

Buchwitz et al [2007] has shown the utility of CO_2 long-term monitoring using SCIAMACHY data. For long-term monitoring per se there are no requirements for auxiliary data. Requirements for auxiliary data for interpretation are similar to the considerations already discussed.

3.5.4 Summary

Sentinels 4 and 5 can provide crucial data for climate applications in inverse modelling, assimilation and long-term monitoring, all of which impacts on protocols.

For the target species themselves, the use of mean dry mole fraction or mean dry air mixing ratio is standard – the product is often denoted as XGas so XCO_2 or XCH_4. The corresponding auxiliary data requirements are for O_2 and CO_2 columns (surface pressure) for normalisation to mean dry air mixing ratios. Hence, there is an extra dimension to CO_2 in that it is used as a normalisation for CH_4 measurements as well as having an absolute importance in its own right; CO_2 is used in preference to O_2 because it can be measured at an adjacent wavelength to CH_4 lowering errors from the wavelength dependence of light. This has been studied in Task 3.

A more diverse aerosol data set including aerosol type is required over and above simple optical depth.

In addition, for assimilation, the direct availability of Level 1 calibrated spectral radiances is a requirement for both core and downstream services.

For auxiliary data for greenhouse gas inverse modelling and for assimilation of greenhouse gases, the most important parameters are fire (burned area), land cover maps, vegetation intensity indication (e.g. FaPAR, Leaf Area Index) for land; ocean colour and sea surface temperature for the ocean; atmospheric chemistry observations which constrain OH. For the CO_2, CH_4 system, OH will be constrained by CO although methyl chloroform is more standard. Note that CO measurements are required for CH_4 inverse modelling since CH_4 and CO are inter-linked.

Meteorological and in situ data sets are the foundation of assimilation and inverse modelling systems and need to be available. It is beyond the scope of this study to improve the meteorological system beyond that intended for MSG/MTG and Metop/post-EPS. There is an issue with measurements of clouds and cloud optical depth, which would improve the climate and air quality applications, particularly for convective clouds.

3.6 Delivery times for air quality information

3.6.1 Introduction to the question of delivery times and their importance

Objectives
Sub-task 2.2 focussed on elaboration of requirements for data delivery times. This work is relevant to considerations on the ground segment within the Phase 0 system studies. As part of sub-task 2.2 activities, scenarios for data processing in the user segment shall be worked out – where possible involving representatives of user organisations.
Delivery time requirements shall be

- based on these scenarios,
- shall be reported for individual applications and
- the needed level of data.

The scope of this activity includes all data (not only auxiliary data).

Thematic specification
As a consequence, the study has to estimate the depreciation of data benefits with increasing delay time for time critical services only. Depending on individual applications, the question of delivery time can be understood in two principally different types:

1. delivery as fast as possible, independent of time of day, and
2. timely delivery at fixed times during the diurnal cycle.

In practice, as a consequence of ground segment infrastructure design, the question can be confined to *diurnal time scale* considerations, that is, how much per day, and when during the day. Applications allowing for lower frequency update cycles than a day are considered as non-time critical and consequently beyond the scope of task 2.2.

3.6.2 Typical users and typical air quality systems

Basically, four different kinds of users may be identified to be reliant on fast data delivery of data envisaged for sentinel 4 and 5 sensors.

- Numerical weather prediction (NWP),
- UV sunburn intensity and times, along with UV indices
- Aviation warning against volcanic dust particles and aerosols
- Air quality forecasts and monitoring.

Another distinction is feasible, that is in terms of temporal understanding

1. timely at some specified hour of the day (hh:mm UTC, ...), or
2. minimal delay from observation time to provision time of user requested output (max ($t_{forecast}$-t_{obs}))
3. revisit frequency (n/(per day)

For the rest of this study mainly items 1 and 2 are of relevance.

3.6.2.1 Numerical weather prediction

Presently, from the viewpoint of atmospheric chemistry, most notably stratospheric ozone and tropospheric aerosols are of interest in NWP: In both cases, radiative budget calculations are considered as of importance for improvements of diabatic process simulations, while applications for wind/transport assimilation by using trace gases and aerosols as air mass markers, are sometimes attributed some future relevance. For the former case of ozone, the positive impact for heating rates can be established by estimation. A direct short term impact of ozone is not likely to be strong, as can be seen from Figure 3-1, although it is nearly as strong as that of scatterometer observations. The effect is more likely to be long-term. In any case, the type of delivery for NWP purposes is of “fixed times during the diurnal cycle”.

3.6.2.2 UV sunburn intensity

Information is required in terms of UV dose forecast and sunburn time forecast in minutes. Transmission to public end users is provided by UV-Check Service (Internet and SMS service) and by daily weather forecast. UV-Check is based on satellite. This relatively new service, as for example implemented in the related section of the GSE PROMOTE, is largely dependent on numerical weather prediction and stratospheric chemistry modelling. Typical applications include short-term advice for the public, most notably during morning hours, usually published by weather services in addition to the standard weather forecast web pages and by SMS. As stratospheric chemical conditions is of importance, with high degree of dynamic control aloft, it can be argued that the time frames given by NWP is timely enough, such that UV sunburn activity does not request special treatment and can be treated as a combination of both air quality considerations and NWP scheduling conditions.

3.6.2.3 Aviation warning against volcanic dust particles and aerosols

Releases of volcanic ashes and aerosols detrimental to aircraft engines are of importance for flight routeing centres, airlines, and weather briefing offices at airports.

3.6.2.4 Air quality forecasts and monitoring

While air quality monitoring via “data fusion” can be taken as the solution of a multi-observation type data assimilation problem, air quality forecasting service is generally based on comprehensive deterministic three dimensional physico-chemical air quality forecast models. The underlying algorithms are solving advection-diffusion-reaction type equations. The use of statistical components is restricted to auxiliary tasks only, like error validation. The forecasts include chemical weather predictions ranging from 3 to 4 days, which are based on driving meteorological forecasts. The envisaged service encompasses integration domains from the European continental scale down to selected European regions and cities by nesting techniques with the following atmospheric constituents considered:

- Ozone
- Sulphur dioxide,
- Nitrogen dioxide,
- Carbon monoxide,
- Formaldehyde (with rarely available in situ observations, but increasing number of tropospheric column retrievals)
- Benzene (with virtually no routine observations)
- particulate matter PM10, PM2.5

Air Quality Index, as an application dependent synthetic measure.

The forecast and monitoring products are given by maps, either synoptic, or as daily maxima or average composites.

3.6.3 NWP and Air quality systems and their operations: current and future

NWP

There is a tight and highly interdependent scheduling system for NWP systems, where sequences of data assimilation, forecasts and increasingly ensemble forecasts only allow for minimal changes. Some considerations relevant to task 2.2 merit special attention, as computational expenses must be traded with reward in forecast skill. As an example for data ingestion in an operational scheme, Figure 3-1 exposes the assimilation and forecast schedule of ECMWF for the midnight forecast. In this figure, a fundamental dilemma of spatio-temporal

data assimilation is addressed. By application of the four-dimensional variational (4D-var) data assimilation technique, an attempt is made to augment the suite of observational data by temporal extension, necessarily to the past, forming assimilation windows of adaptable length. In the case of the ECMWF schedule, a large 12 hours assimilation interval is applied for this purpose. While observations of the temporal evolution assimilated in one assimilation step clearly forces the model as a constraint closer to reality, the effective forecast start is likewise placed backward in time coinciding with the beginning of the assimilation interval. Hence, by starting computationally time demanding assimilation and also including "aged" observations at the beginning of extended assimilation intervals, the benefits of the wealth of observations ingested must be traded likewise with "aged" forecast starts. As a measure to mitigate the consequences, ECMWF selected a two phase procedure, where a long 12 hour assimilation run assures the exploitation of a large suite of data, followed by a short 6 hour assimilation interval, amenable to make use of the most recent observations. It is the latter, shorter assimilation procedure, which provides the initial values for the long forecast, designated for public usage.
For estimating the delivery time limits of sentinel data, operational schemes of users like weather services have to be taken into account, along with estimation of acceptable delays of retrievals.

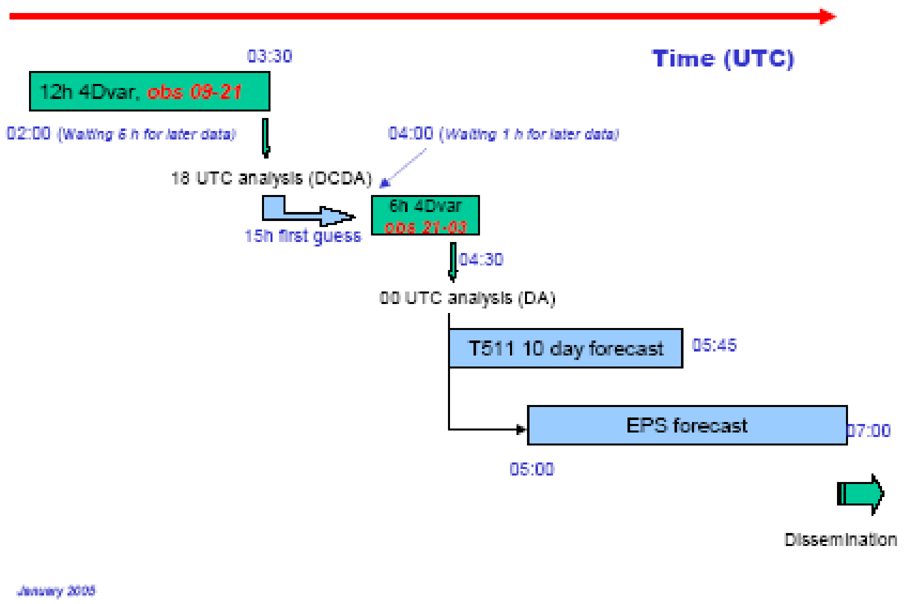


Figure 3-1. The ECMWF solution of the time delivery problem: how to exploit an augmented observational data record (12h) and most recent data (6h), with minimal forecast start delay (4:30), as introduced 2004. Graph taken from Persson and Grazzini, User Guide to ECMWF forecast products, 2007.

Air quality forecast and assimilation based monitoring
Generally, the following basic assumptions are taken to be applicable:

- only NRT requirements engender time critical issues
- two general types of tasks occur:
    1. NRT monitoring of chemical states, and
    2. air quality *predictions of the 1st kind*, that is model initial values are relevant,
- no direct climate diagnosis is requested in a time critical manner.

With the term "*predictions of the 1st kind*" those applications are meant, which do critically rely on initial values for forecasting. It is the data assimilation procedure, which provides updated initial values for the model run from most recent observations. In contrast, forecasts of the 2nd kind only strive for forecasts with the right statistical properties, relying on the pertinent specification of model parameters. Inverse modelling is the corresponding approach to infer these model parameters, which are usually assumed to be stable on a time scale significantly longer than the forecast time span. While in NWP clearly the initial values are of most importance, the emission rates are of like importance, at least, with occasions of strong variations in case of special events. Air quality forecast services are to be provided at all scales as requested by the current directives through nested systems interfacing with each other.

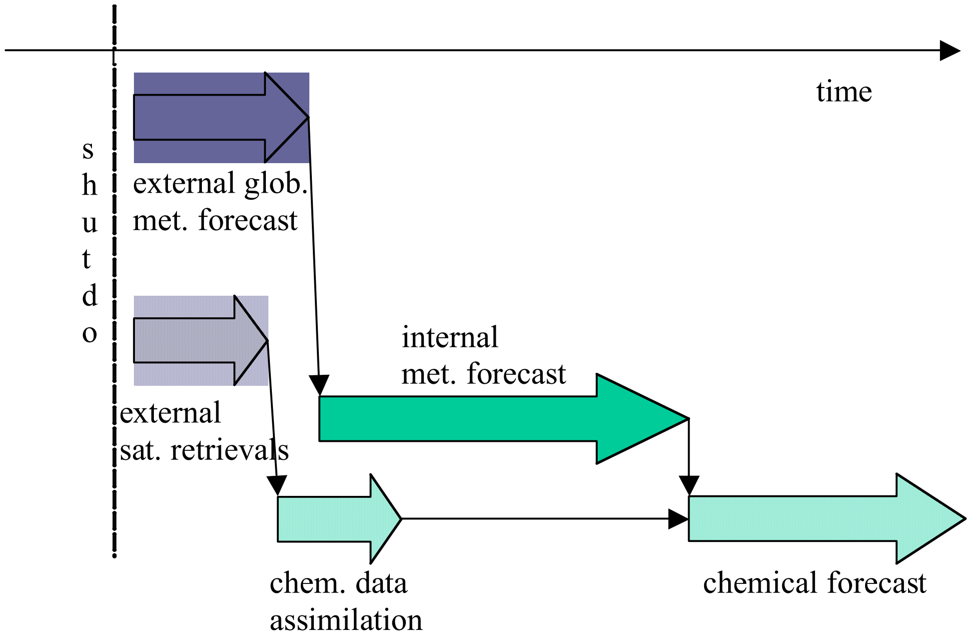
More specifically, the multiscale requirements pertinent to state of the art air quality models Chemistry Transport Models (CTMs) include:

- High resolution air quality forecasting by hemispheric/continental to regional scale (optionally 1 km resolution) nesting techniques with integrated meteorological driver model, allowing for transfer of meteorological data without interpolation,
- Advanced heterogeneous chemistry mechanisms with comprehensive aerosol and photooxidant modules.
- Forecasts tailored to the individual demands of the environmental protection agencies, in terms of focal region, target resolution and species, and visualisation specifications,
- Capacity for routine cross validation of forecasts
- Ability to produce heterogeneous forecast ensembles for error estimates by two different forecast systems, which nevertheless rest on the same modelling principles
- Integrated advanced chemistry data assimilation system.

In general, future directions will consider increasing importance of more sophisticated assimilation techniques and ensemble usage for both assimilation itself and forecast skill predictions. Therefore the ability of the models to ingest satellite data is expected to increase rapidly over the next decade.

As concerns the question of delivery time, the critical issue is the loss of value of information, with progressing time. Principally, this applies for both, observations and auxiliary data, like meteorological forecasts, used either as lateral boundary data or as meteorological driver data. It is therefore possible that, dependent on the most critical issue, two different schemes are to be considered. Figure 3-2 depicts a case where most recent meteorological data supply is crucial (case a), and where most recent chemical data is of importance (case b).

a)



b)

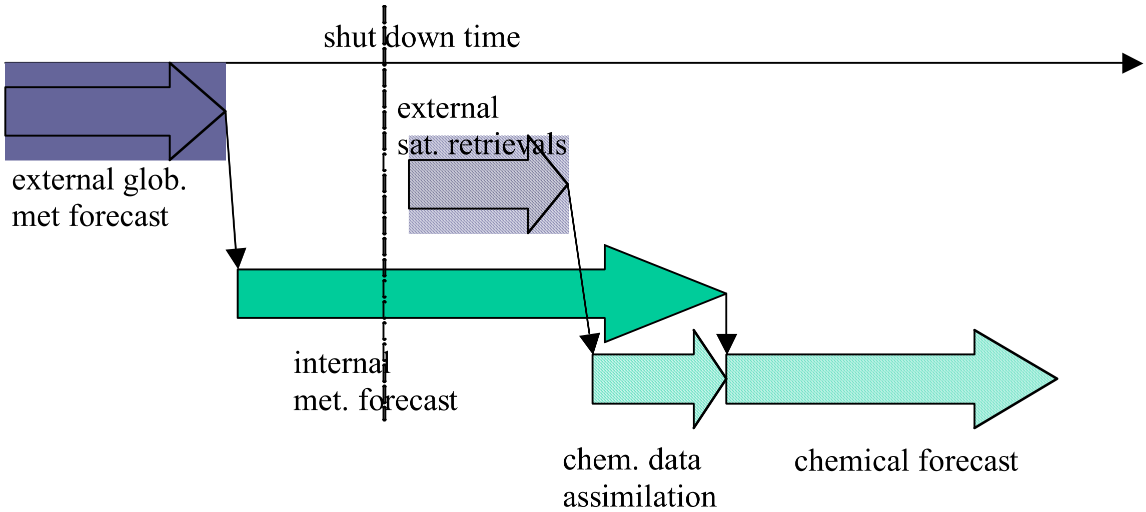


Figure 3-2. *Two processing schemes featuring different relative ageing times of observational data and global meteorological forecast as auxiliary data for regional air quality modelling with internal regional meteorological driver forecast: a) condition where external, that is global, meteorological forecast must not be older than chemical observation time. b) validity of pre-run global (and regional) meteorological forecast is sustained and applicable for later chemistry simulations with chemical data retrieval and data assimilation. Shut down time designates the most recent retrieval, acceptable by the system configuration.*

3.6.4 Results of user survey

Air quality issues are of special importance because the satellite data will directly feed into processing chains with air quality interested end users. This section discusses the air quality demand for data at which specific hour of the day (type 2 as defined in section 1). Two choices appear to be of most significance:

1. if legal action required (e.g. *recommendations, warnings, interdictions*): notice **at the eve** of a critical day, at latest
2. if information for the day required: *early morning* issue

Air quality NRT monitoring and forecast availability is then required by end users with the following remits:

- Environmental Protection Agencies with legal commitments. Official action plans mainly also rest on NRT in-situ data monitoring,
- private users, health concerned,
- commercial users, e.g. route planning for transportation

While delivery as fast as possible, independent of time of day, is a mere technical problem to preserve time critical benefits of any satellite data derived product, the question at which hour of the day satellite derived data products are most useful for environmental protection agencies (EPAs) required consultancy. A limited user survey among cognisant officers of EPAs with satellite data and model use aspirations has been performed. Among possible choices within the scope of non-accidental conditions, the following two turned out to be the key options:

- Early morning air quality forecast:
  - benefit: most recent observations assimilated, predictive skill upgraded, for public information and personal planning,
- Afternoon/evening air quality forecast
  - benefit: timely forecast more amenable for traffic and combustion regulations by authorities.

With the Federal Agency of Environmental Protection (Umweltbundesamt) Austria, the Material Sciences and Technology Institute EMPA in Switzerland as corresponding institution, and the Northrhine-Westfalian State Agency for Environmental Protection, Nature Conservation, and Consumer Protection (LANUV), as official institution in the largest industrialized region in Europe, representative authorities have been contacted.
The results can be abridged as follows:

- UBA Austria, Dr. Robert Höller
  - early morning forecast appreciated, because of higher accuracy of meteorological forecasts
  - warning and traffic regulation issues under the control of federal states, or capital
- EMPA Switzerland, Dr. Dominik Brunner
  - traffic regulation under auspices of cantons
  - 3 level action plan (mainly particulate matter oriented):
    - information level: recommendations to the public
    - intervention level I: fire restriction, speed limits
    - intervention level II: extension of traffic limits
- LANUV Northrhine-Westfalia, Dr. Sabine Wurzler
  - federal and municipal control of measures
  - generally oriented along the lines of Austria and Switzerland

In summary, result of inquiry and experiences within PROMOTE and GEMS indicate:

- For most EPAs, as yet chemical weather prognoses are hardly considered as decision basis, (with the possible exemption of French agencies)
- Presently, often current measurements and meteorological predictions for the next days serve as decision basis of further action
- there is no clearly identified time of delivery in the diurnal cycle. Rather, several dates can be envisaged:

3.6.5 Discussion of results and requirements of delivery time

NWP and UV insolation (and aviation warnings)
It is assumed that, for practical reasons and because of system set-ups of meteorological forecasting systems and global stratospheric chemistry, delivery time requirements for NWP can be combined with UV forecast

generation. It is evident that the delivery category is of type "hour of the day (say, following present ECMWF config.)" with optimal designs to fit for 00:00 and 12:00 UTC forecasts. With this assumption, the estimate is given, that an acceptable delay from observation time to provision time of user requested output (max ($t_{forecast}$-t_{obs})) is about 4 hours, and a revisit frequency (n/(per day) of 2
Todays and surely future forecast skills for UV insolation easily bridge time spans between twice daily forecasts, except small scale cloudiness. It is therefore concluded that *for the specific application of NWP, global chemistry transport modelling, and UV sunburn intensity no challenge for delivery time is posed.*
For aviation warning from volcanic exhaust however, there is a permanent challenge in provision of permanent monitoring results. With increasing time the diffusion of exhaust particulate matter covers larger areas and impediments of air traffic is increasingly likely. First analyses should be available after one hour, in this special case of volcanic eruptions.

Air quality
Notwithstanding the more vague result of EPA representatives' interrogation, in practical terms a key problem can be condensed to the following question:
How fast does the value of retrievals vanish after the overpass of the satellite, when use is intended for time critical applications as described above?
To answer this question a series of assimilation runs and analysis evaluation has been performed, with different processing schemes and differing species dependences

Gas phase information decay
Ozone: The decay of forecast skill after comprehensive data assimilation with the 4D-var technique based on in situ data has been quantified in publications, e.g. in Elbern et al., 2007.
After two data void days most of the information is lost and another assimilation sequence is required to recover the former result. In this case, where ozone assimilation is performed, time critical issues are visible after time spans significantly longer than hours, but smaller than a day.
NO_2: For gas phase chemistry, tropospheric NO_2 column retrievals are meanwhile widely available. As concerns the decay of information time of this highly reactive gas, assimilation runs with satellite retrievals of NO_2 columns were assimilated by both 3D-var and 4D-var. For the latter case, NO2 tropospheric column retrievals from satellite overpasses during the late morning hours can well be reproduced, based on 4D-var assimilation, when the forecast start is at midnight. Worse results are obtained for 3-d var assimilation. Hence, the assimilation procedure plays a key role in preserving retrieval information. Regrettably, the more advanced assimilation methods need considerable computing time, requesting its share in the quest for partitioning of processing time in competition with satellite data delivery time. In any case, the assimilation technique is crucial, to make best and most durable use of data.

Aerosol phase information decay
In order to include a satellite data example for the present study, the combined AATSR and SCIAMACHY aerosol PM_{10} and $PM_{2.5}$ retrievals provided by the SYNAER retrieval procedure wee assimilated in the comprehensive University of Cologne aerosol chemistry transport model EURAD by the three-dimensional variational (3D-var) data assimilation procedure to estimate aerosol decay times. The time span investigated includes a five month period from July to November 2003, including extensive wild fires during the summer period. The area covered is the extended European continental domain. It was possible to validate the persistence time of the assimilation result, showing the beneficial impact of sophisticated data assimilation over a time span of several days in forecast mode. The accumulation of information of aerosol contents is long enough to allow for relaxed delivery times, say up to half a day.

3.7 Summary for Complementary Observations and Delivery Requirements

This study has examined auxiliary data in the context of the target gas and aerosol retrievals, the validation and quality of the system, air quality and climate applications. Overall the results show that the current system likely contains most of the key parameters that are required as a baseline for air quality and climate and the requirements for auxiliary data in terms of instrument capabilities are not high.

The strong conclusion is that very good knowledge of clouds and aerosols is required to meet user requirements. These necessitate use of the O_2 A-band for both air quality and climate monitoring in the UV-visible and NIR/SWIR bands. The use of O_2 A-band is recognised in the MRD and its use is demonstrated in Task 3. For clouds, one can identify cloud fraction, cloud top height/pressure and cloud optical depth; for thermal infrared measurements, cloud top temperature is also required but can possibly be inferred from cloud top height/pressure. Similarly the O_2 A-band facilitates surface pressure measurements.

One crucial area concerns the normalization of column data to mean dry mole fraction or mean dry air mixing ration. This requires the measurement of O_2, O_4 or CO_2 columns as appropriate to reduce uncertainties arising from photon path effects. The CO_2 normalisation is more relevant to the SWIR gases, CH_4 and CO, since the difference in wavelength is least. Hence CO_2 measurements have a relevance also to CH_4 and CO interpretation. In addition, surface pressure is a useful parameter for the system output (from met. analyses or retrievals) although most likely to be insufficient spatial resolution for normalization of columns for pressure variation.

Users also requested the availability of Level 1 calibrated spectral radiances for core service and downstream applications.

Based on a user survey and literature, it is suggested that a satellite product estimating the photolysis rates for NO_2 should be produced. For the photolysis product, aerosol and cloud optical depth are additional data sets, which are required, and these would offer extra capabilities to the air quality model.

Easily accessible daily image data of the MODIS form should be produced to provide near real-time and post-event analysis of pollution events. The requirement for daily image data could be satisfied by Sentinel-3 OCLI and SLSTR. These instruments can also provide desirable datasets on aerosols (with dust separation), fires, land cover and land surface temperatures.

Auxiliary data for air quality and climate had a fair degree of synergy. It was found that the most desirable aspects were aerosol with dust separation, fires, land cover, vegetation intensity (FaPAR, leaf area index) and temperature; ocean colour and sea surface temperature are required for carbon fluxes. Meteorological data are a necessity for many user applications. It is assumed here that these are available through the EUMETSAT and Meteorological organizations. There is an issue with measurements of clouds and cloud optical depth, which would improve the climate and air quality applications, particularly for convective clouds. Atmospheric composition measurements are required to constrain OH. The measurement of CO and NO_2 provides this capability in the first instance and measurements of volatile organic compounds (VOCs) would add to this; methyl chloroform is the current in situ standard.

In-situ data are of high importance for the proper assimilation of satellite data in terms of bias characterisation, inverse modelling significance, validation and quality control.

Overall, the validation auxiliary data looks to be in good shape but some key issues must be addressed and provided that gathered and utilised in an efficient manner. Collection of data and operability are issues that will need to be considered.

The key issues are the accuracy of greenhouse gas measurements achieved by the FTS systems in the NDAC and TCCON networks, the spatial representivity and accuracy of MAX-DOAS systems, and the ties between the remote sensing instruments and the surface in situ network (particularly for air quality). For air quality, urban validation is a significant issue. Excellent progress has been made in recent years and could enable the requisite performance to be achieved by the time of flight of the Sentinels.

The nature of the validation information is likely to be important and at least for some sites knowledge of local site conditions, trace gas variability and stratospheric burdens will be required. Good numbers of coincidences are required for statistical significance to be associated with the comparisons and hence long-term inter-calibrated measurements are required.

Ground segment requirements are for the following data sets: meteorological forecast temperature/ humidity/surface pressure; digital elevation databases; surface albedo/emissivity databases; climatologies of target gases (and their contaminants); spectroscopic databases. In addition, chemical-transport models would be required if VCDs were an output at Level 2.

In summary delivery times for satellite data can be described as follows:

For NWP and UV forecast applications, a delivery time has to adapt to regular service schedules. With estimated 4 hours acceptable delay time for NWP purposes, this is a relaxed condition in comparison to typical meteorological observations, which have to indicate unstable conditions like baroclinic areas or imminent convection. It is expected that from NWP users there is no special challenge for ground segments.

For air quality forecast and monitoring, an estimate from the viewpoint of *direct* end user applications like EPAs is difficult by the following reasons:

- a definitive time of delivery during the day cannot be given, as different purposes call for different hours of preference (for example administrative restrictions to be announced very early, say, at the eve of the forecasted threshold exceedances, while less impacting information is accepted on a short term notice),
- as of today, for EPAs latest measurements and meteorological predictions for the next days serve as a decision basis for further action,
- as yet chemical weather prognoses are hardly considered as decision basis.

However, from the *indirect* viewpoint of data processing by air quality forecasts based on assimilation of satellite data, delivery time estimates are inferred indirectly by assessment of acceptable delay times for beneficial use of satellite data. With this strategy, moderate challenges are given with aerosols and chemical more inert species. Most challenging conditions are found with photo-chemically highly reactive gases like NO_2. In this case, the data processing technique, specifically the sophistication of the data assimilation algorithm, turned out to be of crucial importance. It is concluded, that at least a delivery time of 3 hours maximum allows for time of further processing (assimilation/monitoring and subsequent forecast), resulting in useful information. In the case of ozone and tropospheric aerosols, somewhat relaxed delivery times may be acceptable, with ozone estimated 5 hours and aerosol about 8 hours. In any case, photochemically highly reactive species as NO_2 impose the time limiting conditions. As concerned the hour of delivery, no clear indication of preference could be gained from users. However, with sensors operating in the UV-VIS range, late afternoon delivery is a preferable choice

4 Retrieval Simulations

The purpose of this Task 3 was to consolidate the instrument performance requirements of the MRD. To this end, detailed retrieval simulations studies have been performed, to analyze the uncertainties for different scenarios. The results of these analyses will enable to translate the geophysical observation requirements (Level 2) into instrument requirements (Level 1B). In preparation of the retrieval simulation studies, first the different observation principles for the different species have been documented. Based on this work a selection was made of which observation methods were to be studied in detail. Also, before starting the retrieval simulations the simulation and retrieval tools of the different partners in the project have been modified and/or extended.

Task 3 was set up per geophysical data product. As an example, all retrieval for ozone have been treated as a sub-task and reported together. This approach allowed the trade-off between different observation principles (i.e. comparison of the performance of the UV and TIR in the case of ozone). As a spin-off, this approach has brought together the scientist from different communities (e.g. UV and TIR community) to work together, which provided insight in each others retrieval approaches and resulted in intense co-operation.

For some species, like ozone and carbon monoxide, more than one partner in the CAMELOT consortium has done the analyses. Especially for difficult retrieval problems, like for example the combined retrievals in two spectral ranges, this approach has been very beneficial: it provides much more confidence when the conclusions for complex retrieval problems are supported by two different retrieval approaches.

This chapter contains the following sections:
Section 4.1 presents the selected observation principles.
Section 4.2 describes the simulation tools that have been used in this task.
Section 4.3 compares the expected performance for the different species with the user requirements.
Section 4.4 presents the recommendations for the Level 1B requirements for the UV-VIS-NIR spectral range.
Section 4.5 presents the recommendations for the Level 1B requirements for the SWIR spectral range.
Section 4.6 presents the recommendations for the Level 1B requirements for the TIR spectral range.
Section 4.7 presents the recommendations for the Level 1B requirements for the directional polarization observations.

4.1 Observation principles

The observation principles are the measurements from which the information on a certain atmospheric species is based. The observation principle is a combination of the spectral information (range, resolution and sampling), polarization information, and directional information (number of viewing angles). For most of the trace gases the choices are limited, and therefore the optimal observation principles have been determined from experience and the literature. The selected observation principles, which have been studied in the CAMELOT project, are summarized in Table 4-1.

For most of the species only one observational method has been studied in CAMELOT. Species, for which more than one observation method has been studied, are discussed below.

Table 4-1. Observational principles for Sentinel 4 and 5 studied in the CAMELOT project.

Species	UV-VIS-NIR	SWIR	TIR	Additional observations
O_3	X		X	Combined UV-TIR retrievals. Polarization, multi-directional (LEO only)
NO_2	X			
SO_2	X			
CH_2O	X			
H_2O	X		X	Combined NIR-TIR retrievals
CO		X	X	Combined SWIR+TIR retrievals
CH_4		X	X	
CO_2		X		
HNO_3			X	
N_2O_5			X	
PAN			X	
Aerosol	X	X		Polarization, multi-directional (LEO only). Altitude information from gas absorption bands.
Cloud	X			Altitude information from gas absorption bands

Ozone is a very important species for air quality and climate monitoring. Tropospheric ozone retrieval is challenging because of the large abundance of ozone in the stratosphere, compared to the troposphere, and there is no observation technique that can measure height resolved ozone concentration throughout the troposphere. For this reason ozone was studied in CAMELOT both in the UV, which provides most information in the stratosphere, and in the TIR, which provides more information in the free troposphere. Combined retrievals have been studied to improve the vertical information on ozone for the lower troposphere, including the boundary layer. In addition, limited investigations have been done on the added value of directional and/or polarization information in the UV.

Carbon monoxide and methane were studied in the SWIR and in the TIR. Similar to ozone, combined retrieval of in this case SWIR and TIR can provide more vertical information in the lower troposphere.

Water vapour absorbs in almost all spectral ranges. In the TIR many water vapour lines are available which can be used for measuring a vertical water vapour profile. In the NIR water vapour absorption bands are present that do not provide as much independent pieces of information as the TIR, but may have some advantage over land. Combined TIR and NIR retrievals have been studied to investigate whether water vapour can be measured significantly more accurate using this combined approach.

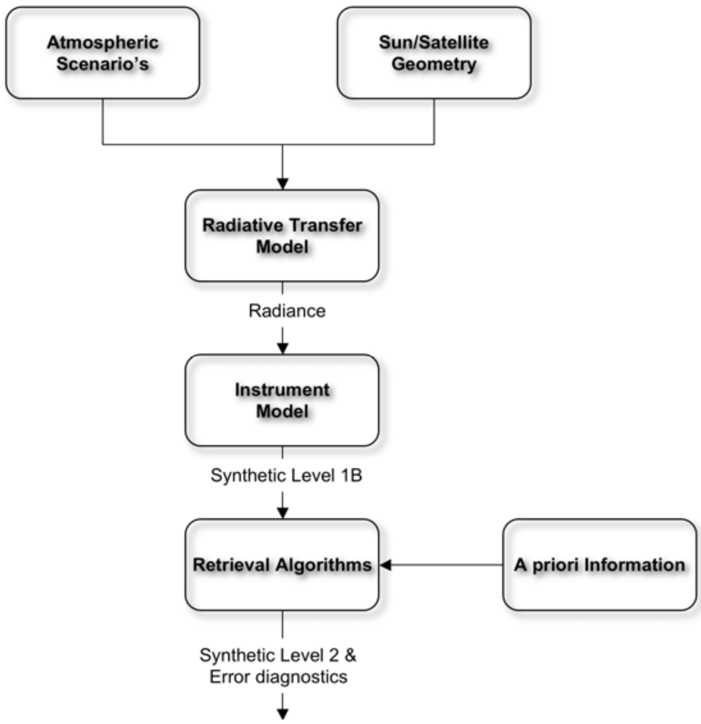
Aerosols have the largest effect in the shortwave part of the spectrum (UV to SWIR). Because of the complex retrieval problems for aerosols, directional and polarization observations are needed to reduce the dependence on a priori information on for example the surface reflectance and the aerosol size distribution. Measurements in gas absorption bands in the NIR and SWIR have been studied to investigate the possibility to retrieve the vertical distribution of the aerosol particles.

4.2 Retrieval and Error Assessment Tools

To perform the Level 2 simulations a chain of tools has been used as schematically shown in Figure 4-1. This chain consists of the following components:

- Atmospheric scenario's:
  Scenario's that have been delivered by the Task 1 activities and consist of profiles of the different trace gases, aerosol profiles, pressure and temperature profiles, etc.
- Sun-satellite Geometry
  Solar zenith and azimuth angles and viewing zenith and azimuth angles applicable for the simulated ground scene. Note that for the TIR retrievals the solar angles are not considered.
- Radiative Transfer Model
  Computes radiance at the top-of-the-atmosphere for a certain atmospheric scenario given the Sun-satellite geometry. Often, derivatives with respect to atmospheric model parameters are also calculated, as these may be needed for the retrieval algorithm and error characterization.
- Instrument Model
  The instrument model simulates the Level 1B using the synthetic radiance as input. These models can have different complexity ranging from an instrument spectral response function and a simple noise model to a full description of the hardware components.
- Retrieval Algorithm
  The retrieval algorithm uses the Level 1B and a priori information as input and derives the synthetic Level 2 data and error diagnostics.

Figure 4-1. Schematic illustration of the different inputs and tools used in the retrieval simulations.



The tools used in the CAMELOT studies are based on existing tools. Adaptations that have been done for CAMELOT include:

- Modifications to interfaces to read the atmospheric scenario's;
- Modifications to the instrument models to cover the necessary ranges in Level 1B requirements;
- Development of tools to bring the results onto the vertical grid specified by the user requirements;
- Adaptation of the diagnostic parameters to be able to compare the results;
- Addition of more a priori datasets.

During the first phase of the study the a-priori variance-covariance matrices that are an essential input for optimal estimation retrievals have bee discussed extensively. The results of the analysis will always depend on the a-priori information. An attempt has been made to use the same a-priori information for certain species. This was not always possible, because the a-priori information can affect retrievals from different spectral regions in a different way. In addition, in several cases the a-priori has been varied to demonstrate the impact of the a-priori information.

A list of tools that have been used in Task 3 of the study is given in Table 4-1. The retrieval algorithms are all *state-of-the-art* with a link to operational satellite instruments.

Table 4-2. Tools used for the Level 2 simulations in the CAMELOT study.

NAME **Species**	**Description**
LIDORT NO_2, H_2CO, SO_2	Linearized discrete ordinate radiative transfer code developed by Rob Spurr (RT-Solutions Inc.), for the UV-Vis-NIR.
MARC H_2O	IFAC-CNR line-by-line radiative transfer code for the TIR
LINTRAN O_3, CO, CH_4, Aerosol	SRON's linearized vector radiative transfer model for UV-VIS-NIR-SWIR-TIR. The model provides the intensity vector field and additionally weighting functions with respect to trace gas concentrations and aerosol properties.
FM2D O_3, Aerosol	RAL model developed initial during ESA UTLS study to simulate 2-d solar+thermal RT. Now extended in EUMETSAT O_2 A-band study to include realistic cloud and aerosol optical property models.
SWIM CH_4	Line-by-line radiative transfer model for the SWIR, and retrieval algorithm based on the Optimal Estimation Method
Atmosphit O_3, CO, CH_4	ULB Line-by-line radiative transfer model and retrieval algorithm based on the Optimal Estimation Method
DISAMAR O_3, H_2O, NO_2, Clouds	KNMI tools for Level 2 simulations, including the LABOS RTM model and an instrument model.
GDOAS NO_2, H_2CO, SO_2	Retrieval algorithm developed and used at BIRA-IASB for GOME, GOME-2 and SCIAMACHY nadir trace gases observations
1DVAR	Optimal estimation method, including information content analysis modules, for the retrieval of atmospheric species and surface properties from spectral radiance measurements
Aerosol retrieval algorithm Aerosol	SRON's algorithm for the retrieval of aerosol properties from satellite measurements of intensity and polarization (both Tikhonov regularization and least-squares).
O_3 profile retrieval Algorithms	SRON's algorithm for ozone profile retrieval using Tikhonov regularization
RAL-GOME-O_3	RAL ozone profile retrieval scheme developed and applied to process full global mission of GOME-1, delivering first tropospheric ozone information from GOME. Adapted in EUMETSAT MSG9.7 micron study to perform synergistic retrieval with IASI or SEVIRI 9.7 micron data.
RAL-O_2A	Height-resolved aerosol retrieval scheme for O_2 A-band, developed during EUMETSAT O_2A study.
ORAC	Oxford and RAL scheme for the retrieval of cloud and aerosol optical properties from uv-vis-nir-tir imager data.
IMLM	SWIR SCIAMACHY retrieval algorithm CO and CH_4 2.3 micron (includes instrument model)

4.3 Expected performance versus user requirements

In this section the expected performance of the species studied in Task 3 are compared to the user requirements from the MRD [Langen, 2008]. First a high level overview is presented in section 4.3.1, followed by sections 4.3.2 through 4.3.18 where detailed information is given per species.

4.3.1 Overview

The expected performance of the Sentinel 4 and 5 instruments for the user requirements of the MRD is given in Table 4-3 and Table 4-4. Although somewhat arbitrary, a subdivision between goal and threshold user requirements has been made per species in these tables. In these tables no priority between species has been included. Table 4-3 compares the expected performance with the threshold user requirements, Table 4-4 with the goal threshold requirements.

As can be seen in Table 4-3, it is expected that for the vast majority of the species the threshold requirements will be met. For SO_2 and formaldehyde performance up to the user requirement would require an unrealistic signal-to-noise ratio for the UVN instruments, for PAN this is the case for the TIR instrument. For CO_2 the user requirement on an individual measurement is very demanding and the GOSAT experience should demonstrate the feasibility of these requirements, which will in any case result in very stringent Level 1B requirements. The usefulness of some of the user requirements is under discussion. For CO the tropospheric and total column requirement of 25% is regarded as quite loose. For several species a requirement of 1.3×10^{15} molecules/cm^2 is used, which for certain species is rather loose (e.g. NO_2, N_2O_5), whereas for species (e.g. formaldehyde and SO_2) this requirement is extremely stringent.

Table 4-4 shows that the goal requirements are only met for a few species.

Table 4-3. Assessment of the expected performance versus the threshold user requirements. Green colors indicate that it is expected that the requirements will be met; red indicates that they will probably not be met; yellow indicates that under special conditions the requirements can be met.

OZONE	Theme B1	Theme B2	Theme C1	Comments
Tropospheric Column	25%	25%	25%	
Total Column	3%	5%	3%	
NO_2	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	
Total Column	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	
PBL	10%	10%	--	Under cloud free condition for polluted cases
CO	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	25%	25%	25%	User Requirement not challenging enough?
Total Column	25%	25%	25%	User Requirement not challenging enough?
CO_2	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Total Column	--	--	0.5%	Requirement seems very demanding. GOSAT should demonstrate the feasibility of these measurements
CH_4	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Total Column	--	--	2%	
SO_2	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Total Column	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	--	Volcanic plumes >1 DU (2.7×10^{16} molec/cm^2) can be detected
CH_2O	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Total Column	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	--	

AEROSOL OD	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	0.05	0.05	0.05	Assuming that the stratospheric OD is known within 0.01 OD Multi-angle and polarization observation are required
Total Column	0.05	0.05	0.05	Multi-angle and polarization observation are required
AEROSOL ABS. OD	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	--	--	0.01	Assuming that the stratospheric OD is known within 0.001 OD Multi-angle and polarization observation are required
Total Column	--	--	0.01	Multi-angle and polarization observation are required
AEROSOL TYPE	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	<10% mis-assignments	<10% mis-assignments	--	Aerosol type is derived from the size and refractive index retrievals
Total Column	<10% mis-assignments	<10% mis-assignments	--	
H_2O	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	--	10%	--	
Total Column	--	10%	--	
HNO_3	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	--	1.3×10^{15} molec/cm^2	--	
Total Column	--	1.3×10^{15} molec/cm^2	--	
N_2O_5 (night)	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	--	1.3×10^{15} molec/cm^2	--	Column for the scenario's is less than the requirement of 1.3×10^{15} molec/cm^2
Total Column	--	1.3×10^{15} molec/cm^2	--	
PAN	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	--	1.3×10^{15} molec/cm^2	--	
Total Column	--	1.3×10^{15} molec/cm^2	--	

Table 4-4. Assessment of the expected performance versus the goal user requirements. Green colors indicate that it is expected that the requirements will be met; red indicates that they will probably not be met; yellow indicates that under special conditions the requirements will be met.

OZONE	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	10%	10%	--	
Free Troposphere	20% VR 1-3 km	20% VR 1-3 km	3% VR 2-5 km	Profile information with a resolution of 6-7 km can be achieved
NO_2	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Free Troposphere	20% VR 1-3 km	20% VR 1-3 km	50% VR 2-5 km	
CO	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	20%	20%	--	
Free Troposphere	20% VR 1-3 km	20% VR 1-3 km	20% VR 2-5 km	Tropospheric information with 5 km vertical resolution can be obtained
CO_2	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Tropospheric Column	--	--	0.5%	

CH_4	Theme B1	Theme B2	Theme C1	Comments
Tropospheric Column	--	--	2%	
SO_2	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	20%	20%	--	
Free Troposphere	20% VR 1-3 km	20% VR 1-3 km	--	
Tropospheric Column	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	--	Detection limit of the order 3 10^{16} molecules cm^2
CH_2O	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
Total Column	1.3×10^{15} molec/cm^2	1.3×10^{15} molec/cm^2	--	
AEROSOL OD	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	0.05	0.05	--	Could be achieved with a high resolution O_2-A band and/or 2 µm band in combination with multi-angle and polarization observations
Free Troposphere	0.05	0.05	--	
Lower Stratosphere			0.05 (1/part column)	
Middle Stratosphere			0.05 (2/part column)	
AEROSOL TYPE	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	<10% mis-assignments	<10% mis-assignments		
Free Troposphere	<10% mis-assignments	<10% mis-assignments		
H_2O	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	--	10%	--	
Free Troposphere	--	20% VR 1-3 km	--	
HNO_3	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	--	20%	--	
Free Troposphere	--	20% VR 1-3 km	--	
N_2O_5 (night)	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	--	20%	--	
Free Troposphere	--	50% VR 1-3 km	--	
PAN	**Theme B1**	**Theme B2**	**Theme C1**	**Comments**
PBL	--	20%	--	
Free Troposphere	--	20% VR 1-3 km	--	

4.3.2 Ozone

For ozone the driving user requirements for this study are the total column (3%) and the tropospheric column (defined as 0-12 km range) (25%). User requirements for vertically resolved information of 1-3 km resolution were not considered, because the vertical resolution in the TIR and UV in the troposphere is at best 6 km. In addition to the total and tropospheric columns the vertical profile information with 6 km vertical sampling has been included in the study. The main observation principles considered in the study are TIR and UV nadir sounding. In addition, combined UV and TIR retrievals have been studied, which is possible with the instruments currently planned for Sentinel 5. Also, multi-angle and polarization observations have been included in the study, to demonstrate the possible added value of such observations.

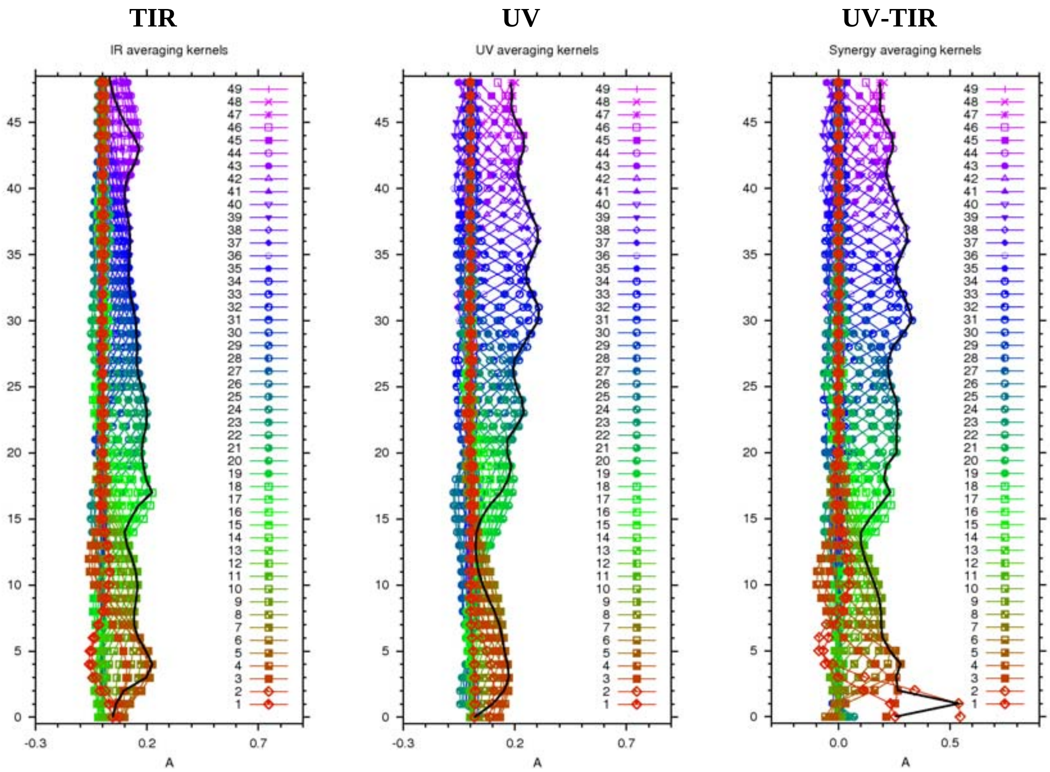


Figure 4-2. The averaging kernels (column of A) and the area (sum of the rows) for ozone for the Tropical biomass burning case with ad hoc a priori of 100% error at all altitudes and a correlation length of 6 km. The plot shows that the combined retrieval contains more information than the TIR and UV separately and has good sensitivity from the surface up to 50 km altitude.

4.3.3 TIR Retrievals

The user requirements for the total and tropospheric column can be met using the TIR observations, both during the day and the night and above all surface types. Current expertise with IASI (0.5 cm^{-1} apodized) demonstrates the possibility of probing accurately tropospheric ozone (0-12 km column, Boynard et al., 2009) and also to detect summer pollution events in the lower troposphere (Eremenko et al., 2008). The potential of IASI to resolve ozone vertical structures in the troposphere and to monitor surface pollution is, however, very limited and highly dependent on the surface thermal contrast. In order to contribute to tropospheric pollution monitoring as required (e.g. through provision of resolved tropospheric ozone profiles) and provided that the radiometric performances are high (typically 0.1 ± 0.05 K), we conclude that the spectral resolution of the TIR sounder should ideally be lower than 0.25 cm^{-1}. Improving on the spectral resolution to ~0.15 cm^{-1} or below would further resolve spectral lines, improve on surface measurements and would enable reaching errors as low as 10-15% on the retrieval of two independent tropospheric columns.

4.3.4 UV Retrievals

The UV wavelength range has been used to build a long-term record on the ozone layer with instruments like TOMS/SBUV, GOME, SCIAMACHY, OMI and GOME-2. In addition to the total column, also vertical resolved information can be derived, due to the strong variation of the ozone absorption in the 270-340 nm wavelength range. The information on the ozone profile contained in the UV spectral range is limited to 6-7 km vertical resolution. Most of the information is in the stratosphere; the spectra contain approximately one piece of information for the troposphere. Hence, the information on ozone from the UV can fulfil only the user requirements on the total column and the tropospheric column. As a consequence, the diurnal variations, which predominantly occur in the lowest few kilometres of the atmosphere, can only be seen for a combination of thick

boundary layers and large ozone concentrations[1] [*Tamminen et al.,* 2009]. Such atmospheric conditions are found over mega-cities during summer. Over Europe this will be limited to large cities in the Mediterranean region and strong pollution events in the summer. Under those conditions, the measurement of the lower tropospheric layer (from 0-6 km) with a high temporal resolution is expected to contain information over vertical transport from the boundary layer to the free troposphere.
To enable the retrieval of the tropospheric column from the UV, the spectral range should cover 305-340 nm. For stratospheric profile information the range of 270 to 305 nm should also be included. For the UV ozone retrieval radiometric calibration is critical. It has to be accurate over a large wavelength range in which the radiance varies by 2-3 orders of magnitude.

4.3.5 UV-TIR Combined retrievals

Within the CAMELOT study the combination of UV and TIR measurements have been studied extensively using a subset of the tested Level 1B performances. This combination can be achieved by using a single L1-2 retrieval algorithm that uses both the UV and TIR information (L1-L1 approach), or by a two step (sequential) retrieval where the L2 product of one of the wavelength regions is used as input for the other L1-2 retrieval (L1-L2 approach). Both options have been studied in CAMELOT.

The idea behind combining the UV and TIR wavelength ranges for ozone retrieval is that they are complementary in terms of vertical sensitivity. The UV spectral range has most of its sensitivity for the ozone profile in the stratosphere and also provides a high level of accuracy on the total column. The TIR spectral range has most of its profile sensitivity in the troposphere and lower stratosphere. Depending on the local thermal contrast between the surface and the lowest atmospheric layers, this spectral range also provides some sensitivity to surface ozone. The simulations in CAMELOT show that combination of UV and TIR is sensitive throughout the atmosphere, from the stratosphere to the boundary layer. Furthermore, the constraint applied to the TIR retrieval in the sequential approach (less variability in the stratosphere and more in the troposphere) enables more information to be extracted from the lowest atmospheric layers, down to the surface. However, and although considerable information is gained in the boundary layer, this is in most cases still not enough to fulfil the user requirements on the column.

The UV-TIR combination is thus a very promising technique for the retrieval of tropospheric ozone, which fully takes advantage of the complementarities of the sounding instruments in terms of vertical sensitivity. However, the current status is that successful retrievals are only shown in simulations studies assuming linearity in the inverse problem, and not with real instruments. Retrieval based on real instruments will be even more challenging because of their radiometric errors, difference in footprint, etc., which obviously require sophisticated error covariance matrices to be built in different domains (horizontal, vertical, spectral…) to provide meaningful results. Scientific studies in the coming years (e.g. IASI/GOME-2) are expected to show if the theoretical gain of combined UV-TIR ozone retrieval can be achieved in practice.

In light of these results and the lack of maturity in data integration and fusion, we do not recommend driving any mission requirements on the combined retrieval technique, which has not yet fully proven its capabilities. *Spectral and radiometric Level 1B requirements should be optimized considering only the capabilities of the individual sounders to probe ozone (see above). We do strongly recommend, however, including in the Sentinel 4-5 missions the UV-TIR spectral ranges needed for the combined retrievals of ozone, which offer theoretically significant improvements in the troposphere and the PBL.* For that purpose, the spatial co-alignment between the UV and TIR pixel should be of the order of a few kilometres, matching the expected ozone tropospheric variability. Temporal requirements are of the order of a few minutes.

4.3.6 Multi-viewing and Polarization

Within the Sentinel MRD, retrieval of tropospheric ozone is foreseen from measurements in UV and from measurements in the TIR. Another interesting option that has been studied would be to use multi-viewing angle and/or polarization measurements for the retrieval of tropospheric ozone from the UV.

Measurements of relative Stokes parameters $q=Q/I$ and $u=U/I$ in the wavelength range 310-330 nm show a sensitivity to the ozone profile that peaks in the troposphere. Simulations point out that the error on the

[1] This result was obtained with retrieval simulations for the ESA ONTRAQ project.

tropospheric ozone column (0-10 km) can be reduced from 30-40% for the case that only measurements of *I* are available, to 10-30% for the case that measurements *I*, *q*, and *u* (in one viewing direction) are available. A limitation of the use of polarization measurements in one viewing direction is that the information content depends on solar and viewing geometry. Here, polarization measurements hardly add information for single scattering angles close to 180° (exact backscattering direction) and add maximum information for scattering angles close to 90°. The dependence on geometry can be significantly reduced when the same ground pixel is observed at multiple viewing angles. Such measurements contain information on tropospheric ozone because at small viewing angles (close to nadir) more light that is measured by the satellite instrument originates from the troposphere than at large viewing angles. Thus a combination of these measurements helps to separate tropospheric ozone from stratospheric ozone. We investigated the capability of such measurements for an instrument that performs measurements of *I*, *Q*, and *U* at 3 viewing angles (5°, 30° and 60°) in the spectral range 300-320 nm at a spectral resolution of 1 nm. For such an instrument, accuracy on the tropospheric ozone column in the range 8-12% can be obtained. This means that the error is reduced by a factor of 3 compared to radiance-only measurements of a GOME/SCIAMACHY/OMI type of instrument.

4.3.7 Nitrogen Dioxide (NO_2)

Nitrogen dioxide (NO_2) shows strong and highly structured absorption bands in the UV-VIS region from approximately 350 to 550 nm. The interval from 425 to 450 nm is generally used as a baseline for accurate atmospheric NO_2 column retrieval using the Differential Optical Absorption Spectroscopy (DOAS) technique. The absorption by NO_2 is relatively weak; therefore no vertical resolved information is available in the radiance spectra. Because under polluted conditions the amount of NO_2 in the lower troposphere is much higher than in the free troposphere and the stratospheric column can be modelled with sufficient accuracy, the tropospheric column, which is mostly sensitive to the boundary layer, can be observed. In this study the user requirements for the total and tropospheric column of 1.3×10^{15} molecules/cm^2 and a maximum error of 10% for the boundary layer column have been considered. Under polluted conditions, NO_2 shows strong diurnal variation, which is closely linked to the diurnal variation in the sources. For example, during weekdays the NO_2 concentration is larger than during weekends and during the weekday morning rush hour the NO_2 exhibits a peak. Such weekly and diurnal cycles will be observed from the proposed UVN instrument on the geostationary Sentinel 4 mission.
The measurement of NO_2 will be driving Level 1B requirements in the visible wavelength range for the UVN instrument. To fulfil the user requirements of 10% error in the boundary layer NO_2 for polluted conditions, the signal-to-noise ratio should be on the order of 1500. Also, other requirements including those for spectral calibration and spectral features will be driven by the measurement of NO_2.

Apart from the instrumental errors, the tropospheric NO_2 column is sensitive to errors on clouds, aerosol load, surface albedo, and vertical profile shape. In this study, novel techniques have been developed to reduce the errors due to clouds and surface albedo, by combining the retrievals in the O2-A band and the visible wavelength range. Although this method has not been demonstrated on real data (i.e. from OMI, SCIAMACHY or GOME-2), the results are very promising. To enable such combined retrievals, good co-alignment must be achieved between the VIS and the NIR channels.

4.3.8 Carbon Monoxide (CO)

For carbon monoxide (CO) the driving user requirements for this study are the total column (25%) and the tropospheric column (defined as 0-12 km range) (25%). Requirements on the PBL and vertically resolved information in the free-troposphere with a 1-3 km resolution cannot be achieved due to the limited vertical information in the measurements. However, separation of the lower troposphere, where the sources of CO reside and the free troposphere, important for the long-range transport of CO, has been considered in this study. The user requirements for the total and tropospheric column of 25% are considered to be relaxed by the study team. It is therefore recommended to re-assess these requirements; for the Sentinel 5 mission a requirement of better than 15% is within reach.

In this study, Level 1B requirements have been derived from CO for the TIR and SWIR wavelength ranges. In addition to single TIR or SWIR retrievals, the combined TIR-SWIR retrievals have been studied extensively. The TIR and SWIR show strong synergy, where the TIR can bring the vertically resolved information and the SWIR the sensitivity to the total column, including the boundary layer.

4.3.8.1 TIR

Vertically resolved carbon monoxide profiles could be retrieved from TIR radiances during day and night and above land and oceans; considering all or a subset of the carbon monoxide 1-0 vibrational band. The 2140-2180 cm^{-1} interval prescribed in the MRD appears to be well suited for the carbon monoxide retrievals as it allows reaching both high vertical sensitivity and low errors (around 5% on the tropospheric column and 10-15% on average for the PBL). The number of independent pieces of information (DOFS value) on the carbon monoxide vertical structure that can be retrieved from the TIR radiance measurements is 2.5 on average, but depends upon Level 1B specifications: DOFS from 1.5 to 3.5 are obtained when going from the best to worst instrument pairing [FWHM / NeDT]. The estimated vertical resolution is 6 km, which is coarser than the Level 2 requirement but which nevertheless enables capturing vertical variations in the CO profile. Basically, achieving a significant vertical resolution implies relatively stringent spectral resolution requirements. The sensitivity to the ground varies from case to case, and in particular as function of surface thermal contrast.

The error on each altitude level of the retrieved carbon monoxide profile is around 10% from 2 km to higher altitudes. It is strongly dominated by the smoothing error, with some additional contribution from the measurement noise. Additional error sources, originating from uncertainties in fitted model parameters or the temperature profile, are found to be marginal.
The errors on the total column are smaller than 10%, i.e. well below the 25% level 2 requirement. The error on the tropospheric column is similar. However, as stated above, this requirement appears to be rather loose, comparable to the difference between a given regional scenario and global mean *a priori*.
Lower tropospheric column (0-6 km) retrievals can be achieved with an error around 10% with sufficiently high spectral resolution (FWHM smaller than 0.25 cm^{-1}) and low noise (typically NeDT < 0.1 K). At the same time, such a design allows retrieving the upper tropospheric ozone column with a 5% error.
The errors on the boundary layer vary between 10% and 20% depending on spectral resolution and radiometric noise. In case of less favourable thermal contrast values (see below), it reaches 25% but still remains of the order or below the Level 2 requirements.

4.3.8.2 SWIR

The SWIR retrieval of CO is performed in the wavelength range 2305 to 2385 nm. Under clear sky conditions with low to moderate aerosol load, the scattering in the atmosphere in this wavelength range is small and the signal at satellite level is dominated by reflection on the Earth surface. For this reason, this wavelength is uniformly sensitive over the altitude range of the troposphere and thus has the advantage of having sensitivity from the boundary layer to the stratosphere. Due to its dependence on the surface reflectivity, the retrievals are limited to the continents. Apart from scenes that contain low-level clouds, retrievals cannot be performed over the ocean. The lowest surface reflectivities for which retrievals can be performed are directly linked to the signal-to-noise requirement in the SWIR.
The CO total column can be retrieved with an accuracy of approximately 15%, which is much better than the user requirement of 25%.

4.3.8.3 SWIR-TIR Combined Retrieval

TIR retrievals contain vertical information on the CO profile (up to 3 independent tropospheric subcolumns), both during day and night and over sea and ocean. The sensitivity of the TIR instruments to the PBL is however moderate to very weak, depending on local surface thermal contrast situations. The combination of SWIR and TIR greatly enhances the vertical sensitivity near the surface in cases where TIR measurements have very weak sensitivity to that layer. The chief gain of the coupling lies therefore in the identification of continental source regions (surface emission and pollution) with low thermal contrast, such as mid-latitudes in wintertime.

The benefit of the coupling has not yet been demonstrated with real measurements and is in fact not applicable to any current satellite mission, due to lack of complementary sounding instruments in orbit. Spectral and radiometric Level 1B requirements should therefore be optimized considering only the capabilities of the individual sounders to probe carbon monoxide (see above). We do recommend, however, to include the SWIR-TIR spectral ranges needed for the combined retrievals of CO, in order to enhance the mission outputs related to the measurement of PBL pollution in the cases where the TIR sounders are weakly sensitive. This synergy will enable the observations of the sources located at the surface, as well as the long-range transport of CO in the free troposphere.

4.3.9 Methane (CH_4)

The user requirements for methane (CH_4) are driven by the climate application and are given as 2% for the total and tropospheric column. The tight user requirement enables the monitoring of trends in sources against a large background value. Because of the interest in the methane sources the measurement technique should have sensitivity down to the boundary layer. The primary technique that has been studied for methane is the SWIR, which shows the preferred uniform sensitivity at all altitudes, due to the limited scattering in the atmosphere for cloud-free scenes. In this study a trade-off has been made between the following SWIR spectral bands:

- 1.6 µm band (proxy)
- Combined 2.3 µm band + NIR (2 band)
- Combined 1.6 µm and 2.3 µm band + NIR (3 band).

4.3.9.1 Proxy Approach

From these methods the single 1.6 µm band retrieval has heritage in methods used for SCIAMACHY. Although SCIAMACHY also measures the 2.3 µm band, the performance of this methane retrieval is not good enough to meet the user requirements. In the current SCIAMACHY retrievals a so-called proxy method is applied. This method derives the ratio of methane to CO_2 from the 1.6 µm band and computes the methane concentration by multiplying this ratio by the CO_2 concentration from a model, thus using CO_2 as a proxy. The advantage of this method, as also shown in this study, is that it is less sensitive to the presence of thin cirrus clouds and aerosols. However, it assumes that the vertical profile shapes of CO_2 and CH_4 are the same and puts a strict requirement on the knowledge of CO_2 of better than 1%. An additional advantage of this method is that it is a simple algorithm.

The combination of the 2.3 µm and the NIR band uses the O_2-A band for providing information on thin cirrus clouds and aerosols. The advantage of this method is that methane is derived directly from the spectrum, without using auxiliary information on CO_2. The primary disadvantage is that it is more sensitive to cirrus clouds and aerosols.

The combined 1.6 µm, 2.3 µm, and NIR band approach uses the O_2-A band primarily for information on clouds and aerosols. Additional information on the micro-physical aerosol and cloud parameters can be gained from the two SWIR bands. The methane information comes from both the 1.6 µm and 2.3 µm bands. Like the 2.3 µm and NIR band combination, it does not rely on auxiliary CO_2 information. This method has been developed for the retrieval of CO_2 from OCO and GOSAT and adapted for the retrieval of methane. As illustrated in Figure 4-3 this method shows the least dependence on aerosol and clouds.

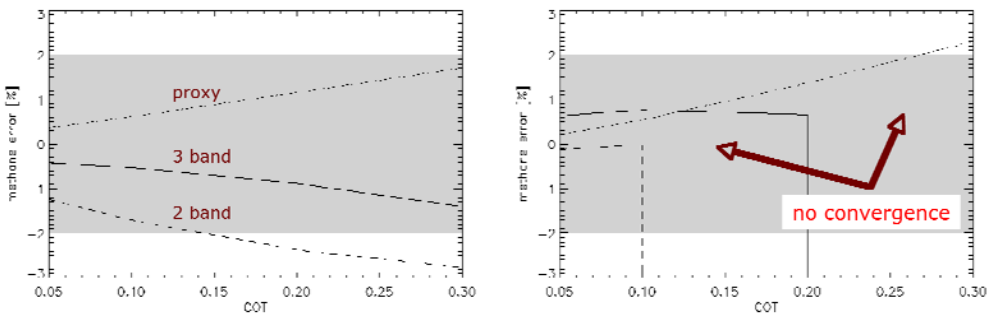


Figure 4-3. Error in methane in % as a function of the optical thickness of a cirrus cloud for 30 degrees solar zenith angle (left) and 60 degrees solar zenith angle (right). The grey area indicates the user requirement. For the proxy method the error in the CO_2 column has not been considered.

Having a 1.6 µm band in addition to a 2.3 µm band is recommended as priority 1 for the following reasons:

- It decreases the error due to aerosols and thin cirrus (both the proxy and the 3 band method);
- The three band retrieval can be verified using the proxy method;
- The proxy method allows for consistent time series with SCIAMACHY.

Besides the trade-off between the SWIR bands, the retrieval of methane also relies on a good cloud clearing method, which selects only the cloud-free scenes or scenes with thin cirrus (optical thickness less than 0.3). For this purpose a cloud imager with bands in the VIS and NIR and a spatial resolution of the order 1 km is needed. The measurements of the cloud imager have to be performed within 1-2 minutes of the SWIR measurements.

4.3.10 Aerosol

The user requirements for aerosols are given in terms of the aerosol optical depth, aerosol absorption and the aerosol type. Requirements are given for the total column as well for sub columns, indicating that there is an interest from users in vertically resolved information. Aerosol type is not a well-defined parameter. In this study we have translated this into requirements for the aerosol size distribution and refractive index. Two observational principles have been studied: a multi-viewing polarization instrument and the use of oxygen, CO_2 and water vapour absorption bands. These observations are complementary: the multi-viewing polarization instrument aims at deriving the total column values for parameters like the aerosol optical depth, size distribution and refractive index, whereas the absorption band methods provides relative information on the vertical distribution of the aerosol.

For the multi-viewing polarization instrument a simulation setup has been chosen that uses little *a priori* information on the aerosol size distribution and composition. The simulations show that single-viewing angle measurements of intensity do not meet the requirement on aerosol optical thickness (or other aerosol parameters), even if the surface reflection properties are perfectly known. If aerosol and surface properties are retrieved simultaneously, multiple-viewing measurements of intensity barely meet the requirement on aerosol optical depth and effective radius, and do not meet the requirement for the refractive index. Multiple-viewing-angle measurements of intensity and polarization meet the requirement on aerosol optical depth and other parameters under all conditions. Therefore it is recommended to add Level 1 requirements for a multi-viewing angle polarization instrument to the MRD. As a starting point for these Level 1B requirements, the 3MI instrument specifications as studied by the EUMETSAT post-EPS group have been used. An assessment of these requirements is given in section 4.7.

For the retrieval of the vertical distribution of aerosol using the absorption bands of oxygen, CO_2 and water vapour, the NIR channel and optionally the 2 µm band are needed. This will result in more stringent requirements on the spectral resolution and noise of the O_2-A band. Retrieval from H_2O and CO_2 bands near 2 µm seems very promising but this is a less mature technique and further work would be required to raise the priority of this channel above the O_2-A band sounder. Using only information from the 2 µm CO_2 band gives similar performance to the O_2-A band sounder in terms of optical depth measured in the respective spectral regions, but it should be recognised that in most conditions the actual aerosol optical depth will be larger at shorter wavelengths and so the shorter-wavelength band is expected to prove more useful. If both channels were present, height-resolved information on aerosol type and size could be obtained, but this is beyond the scope of Sentinel 4 and 5 at present. It is also noted that good temperature profile information is required, so observations must be co-located with those of an IR temperature sounder with capability at least matching that of IASI. As individual and even neighbouring scenes must be completely cloud free, co-location knowledge is not critical.

4.3.11 Clouds

In the MRD no specific requirements are given for cloud parameters, because it is not considered a primary Level 2 product for the Sentinel 4-5 missions. For the retrieval of trace gases in the UV, VIS and SWIR accurate information on cloud fraction, height and optical thickness is needed. To fulfil these requirements a NIR band covering the O_2-A band is included in both Sentinel 4 and 5. To derive the Level 1B requirements for this band, the effects of NO_2 tropospheric column retrieval on the NIR band specifications have been studied. The NO_2 is affected by the NIR band specifications through the cloud parameters that are derived from this band. NO_2 has been selected for this purpose, because it is known to be strongly affected by the presence of clouds and because

most of the NO_2 in the troposphere is situated below two kilometres. The effects of clouds on NO_2 are much larger than for tropospheric ozone.
In this study a novel technique has been developed which uses the NIR and the VIS bands together to derive the cloud parameters, the surface albedo and the NO_2 column. While it has been used to derive the Level 1B requirements for the NIR, it will also reduce the error in NO_2 for cloud-free and partly cloudy situations, as illustrated in Figure 4-4. Although this method shows very promising results, it has yet to be demonstrated using real data.

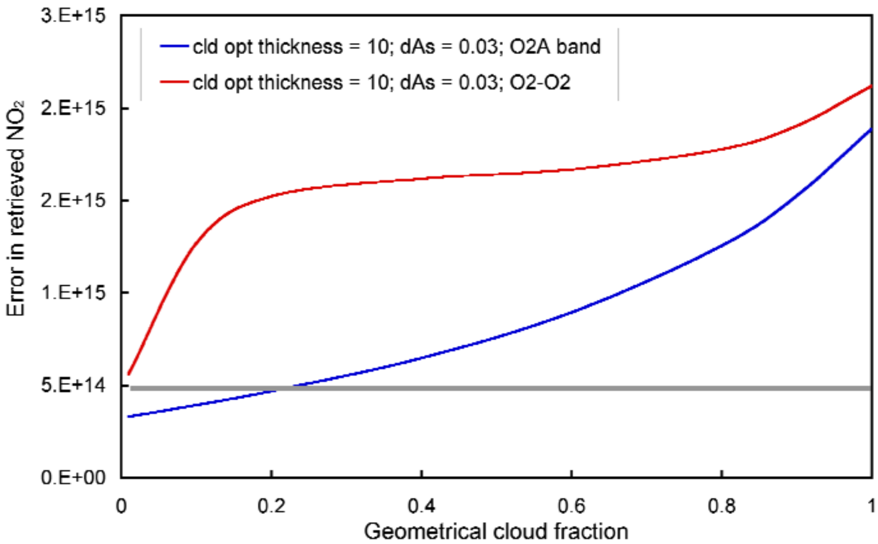


Figure 4-4. Error in the retrieved boundary layer NO_2 as a function of the cloud fraction for a cloud of optical thickness 10. The cloud parameters were fitted using the O_2-O_2 absorption band around 470 nm (red line) and using the O_2 A-band (blue line). The grey horizontal line indicates the user requirement of 10% of the PBL column. The O_2 A-band allows fitting of not only the cloud parameters, but also the surface albedo, for which an a-priori error of 0.03 is assumed. The figure shows that for clear and partly cloudy conditions the newly developed O_2 A-band method reduces the error in NO_2 by a factor of 1.5 to 3.

4.3.12 Sulphur Dioxide (SO_2)

The user requirement for sulphur dioxide (SO_2) for the total and tropospheric columns is 1.3×10^{15} molecules/cm^2 (0.05 DU) and its main application considered in the MRD is air quality. It is noted that SO_2 is also used operationally for monitoring of volcanic plumes, which leads to more relaxed requirements. The user requirement of 1.3×10^{15} molecules/cm^2 corresponds to a concentration of 0.6 ppb, assuming a 1 km thick boundary layer. Air with a lower SO_2 concentration can be considered as non-polluted. From the CAMELOT predecessor study CAPACITY, the 0.05 DU concentration was found to be required to observe the SO_2 gradients indicative of pollution sources. From the study described in this chapter, this value seems to be an unrealistically low detection limit. It has been found that for a realistic signal-to-noise scenario, a detection limit on the order of 3 DU slant column density (corresponding to approximately 1-2 DU total column) is feasible when an optimized fitting window is applied (found to be 310-320 nm) and the solar zenith angle is relatively small. Although the user requirement is not within reach, such a detection limit will enable the monitoring of large pollution sources, such as power plants in former Eastern Europe and industrial regions in China. The Sentinel 4 and 5 spatially and/or temporally averaged SO_2 data will be useful to monitor such regions. Over Europe the diurnal variations in SO_2 that could be observable are driven by emissions from power plants in former Eastern Europe.

One of the difficulties of the retrieval of SO_2 is the interference of ozone. In this study DOAS was used as retrieval method. An optimal estimation technique that fits both ozone and SO_2 may be more appropriate and could enable the shorter wavelengths, but greater than 305 nm, for which the absorption features are large. However, this technique will not be able to bring the user requirements within reach.

4.3.13 Formaldehyde (CH_2O)

For formaldehyde the user requirement considered in this study is 1.3x10^{15} molecules/cm^2. This requirement is extremely challenging, given that the detection limit for formaldehyde from existing instruments is on the order 5x10^{15} molecules/cm^2. Retrieval simulations have been performed for the wavelength range between 328.5-346 nm. These simulations show that approaching the user requirement for individual measurements will result in unrealistic requirement for the signal-to-noise ratio for the instrument. This is in agreement with experience from existing instruments, which show large noise on individual measurement and are usually used after averaging multiple measurements temporally or spatially. Such measurements do contribute to the knowledge of formaldehyde sources and atmospheric processes, and this is also expected from the formaldehyde measurements from the Sentinel 4 and 5 missions. The geostationary observations from Sentinel 4 will have the advantage that ground pixels can be averaged over one day, which also effectively reduces the noise.

4.3.14 Carbon Dioxide (CO_2)

The user requirements for CO_2 of 0.5% for the total and tropospheric columns on individual measurements are recognized as being extremely stringent. Even for dedicated missions like OCO and GOSAT the requirements were formulated to be less stringent. In this study CO_2 has been treated as a lower priority species. The rationale for this choice is that space based observations of CO_2 should first be demonstrated by dedicated mission like GOSAT. The Level 1B requirements derived for CO_2 should be considered as a first assessment.
Retrieval simulations have been performed for SWIR CO_2 channels using the OCO retrieval formulation. Best precision is obtained using both the weak CO_2 band at 1.6 µm and the strong CO_2 band at 2.0 µm. However, use of the strong CO_2 band brings some increased sensitivities, for example, with respect to interference errors due to the presence of finite aerosol layers, uncorrelated to other layers.
The results are very encouraging and suggest that implementation of either or both CO_2 channels is feasible and will yield good accuracies close to 1 ppmv or better. If only the weak band of CO_2 is implemented, then improved noise could be desirable depending on the precision required at a single point. For both cases, performance of the O_2-A band is important, in particular with respect to instrument line shape knowledge and spectral resolution. For both cases, but particularly for the strong CO_2 band at 2.0 µm, knowledge of aerosol layers is important. Hence further rationalisation of the O_2-A band performance will come in synergy with aerosol retrieval work.

4.3.15 Water Vapour (H_2O)

The user requirements for water vapour are driven by air quality applications and include requirements on the total column (10%) as well as sub columns (10%, 20% for free troposphere). In this study the user requirements for water vapour have been treated as lower priority, thus water vapour should not drive instrument requirements. The spectral regions that have been studied are TIR, NIR and a combination of TIR and NIR.

4.3.15.1 TIR

The retrieval of water vapour vertical distribution from nadir viewing measurements in the infrared region is generally based on the exploitation of the strong vibro-rotational features of the water vapour spectrum, particularly in the vibrational ν_2 band at 6.3 µm, which is partly covered by the bands selected in the MRD. The vertical profile is retrieved with a resolution better than 3 km and a retrieval error less than 20% in the free troposphere with the exception of the uppermost layers (typically above 10 km). In some cases, the retrieved profiles below 2 km are affected by a bias of the order of 5-10% (e.g., in the case of the European background and European polluted scenarios). The error on the retrieval of total, tropospheric and PBL column varies from 2% to 5% depending on the geophysical scenario, with both total and partial columns values generally retrieved within the required uncertainty (10%) for most of the scenarios. The occasionally reduced capability to properly retrieve the water vapour content at the lowest levels may introduce a bias in the retrieved columns, with overall L2 performances that, in any case, remain compliant with the 10% threshold fixed by the user requirement.

4.3.15.2 NIR

For the retrieval of water vapour in the NIR a wavelength range of 715-720 nm has been selected. Although different windows are possible, this window was selected because it is close to the O_2-A band, while its performance is as good as or better than other options. The retrieval provides useful values for the total water vapour column and also some information about the vertical distribution. Between 1.6 and 3.5 degrees of freedom of signal (DOFS) are available for the VMR profile, while the largest number of DOFS is found for large values of the solar zenith angle and the viewing zenith angle. The measurement is sensitive to the VMR profile below 6 km, whereas the profile at higher altitudes is determined mainly by the *a priori* profile. The estimated accuracy ranges from 5% for the PBL to larger than 10% above 6 km and can fulfil the user requirements for the total column.

4.3.15.3 NIR-TIR Combination

The wavelength range of the VIS/NIR portion of the combined retrieval is 715-720 nm and fits within the requirements for a UV-VIS/NIR sounder instrument with a wavelength range of 710-750 nm (LEO VIS-3 Band). The spectral range of the TIR portion of the combined retrieval presented here spans 1280 to 1360 cm^{-1}. The simulations indicate that it is advantageous to combine information from NIR and TIR because each individual retrieval is sensitive to different regions of the atmosphere. The TIR retrieval provides critical information for the free troposphere, but has difficulties in accurately measuring the PBL sub column due to problems related to the thermal contrast at the surface. NIR is very sensitive to the lower atmosphere, particularly the boundary layer and is not adversely affected by near-surface thermal contrast scenarios.
Based on the TIR-alone and NIR-alone studies it is reasonable to compare the column and sub column error performance of the combined retrieval to each of the individual TIR and NIR retrievals. For the geophysical scenarios tested, the combined NIR-TIR retrieval has reduced error in both the total column and PBL sub column as compared to the NIR-alone and TIR-alone retrievals. The errors are reduced to values far below the user requirement threshold value of 10%. These simulation studies for the VIS/NIR-TIR combined retrieval show the great potential for providing accurate column and sub column water vapour data and may also be of interest for meteorological applications, but have not yet been proven with real measurements.

4.3.16 HNO_3

HNO_3 can be retrieved in the TIR band between 840 and 920 cm^{-1}. The retrieval simulations performed in this study indicate that sensitivity to the lower atmosphere for the HNO_3 retrieval requires higher spectral resolution and low radiometric noise. The HNO_3 total column retrieval meets the specifications best for 0.125 cm^{-1} resolution and 0.05 to 0.1 K noise using the Europe background retrievals as the standard case. From the range of profiles used in these investigations, scenarios that depict pollution events, such as the tropical biomass burning or the China polluted case, yield the largest gain in information.

In terms of meeting the MRD requirements, the total and tropospheric column errors calculated for the given CAMELOT scenarios can be brought close to the $1.3x10^{15}$ molecules/cm^2 uncertainty value if the instrument specifications are adjusted as recommended for HNO_3.

4.3.17 N_2O_5

N_2O_5 can be retrieved in the TIR band between 1230 and 1260 cm^{-1}. The retrieval simulations performed in this study for N_2O_5 have shown that even at the highest spectral resolution (0.125 cm^{-1}), there is no tropospheric sensitivity as seen from the behaviour of the averaging kernels. From these results, it can be seen that an improvement from the MRD instrument specification makes little difference to what is achievable for the retrieval of N_2O_5. Most importantly, these results show that gaining any sensitivity in the troposphere is not possible and only stratospheric sensitivity can be achieved. This is in agreement with the experience with IASI, for which tropospheric N_2O_5 has not been observed.

4.3.18 PAN

PAN retrieval simulations have been performed for the spectral range between 780 and 810 cm^{-1}. The retrieval simulations presented for PAN have shown that at highest spectral resolution (0.125 cm^{-1}), the DOFS will exceed 1 and even more so when looking at enhanced PAN events. Lower atmosphere sensitivity for the PAN retrieval requires higher spectral resolution and low radiometric noise. The PAN total column retrieval is closest to meeting the user requirements when assuming 0.125 cm^{-1} resolution and 0.05 K noise and using the Europe background retrievals as the standard case. The requirements are however not met for background and heavily polluted scenarios.

4.4 Level 1B requirements UVN

4.4.1 Introduction

In this section regarding the conclusions on the Sentinels 4 and 5, the Level 1B requirements are given. These conclusions are given as recommendations for the MRD Level 1B requirements. These conclusions are primarily based on results obtained using the retrieval simulations performed in CAMELOT Task 4. In addition, some results of the ESA ONTRAQ study Task 3 [*Tamminen et al.,* 2009] have been included where applicable.

4.4.2 LEO-UVN Requirements

The UVN is used to measure the concentration of several trace gases and in additionally provides information on aerosols and clouds. As summarised in section 4.3, the trace gases in the UV-visible for which the user requirements can be met are ozone, NO_2 and water vapour. In addition, the cloud parameters compliant with the ancillary data requirements can be measured. Measurements of SO_2 and formaldehyde cannot meet the user requirement for individual measurements. However, the measurements for these gases can be averaged in space and time to provide information on emission sources, thus indirectly contributing the air quality and climate themes. To provide aerosol information compliant with the user requirements, more than one viewing and/or polarization measurements are needed, in combination with a higher spatial resolution, to avoid cloud contamination. The UV-visible also provides extra information on aerosol absorption and potentially aerosol height from the O_2-A band.

4.4.2.1 Geometrical Requirements

MRD Requirements: MR-LEO-UVN-1, MR-LEO-UVN-2, MR-LEO-UVN-3, MR-LEO-UVN-4, MR-LEO-UVN-5, MR-LEO-UVN-6, MR-LEO-UVN-7, MR-LEO-UVN-8

The LEO-UVN instrument should measure the Earth radiance continuously, without gaps between the ground pixels. This is achieved when the spatial sampling is less than or equal to the spatial resolution. The instrument should provide daily global coverage, meaning that the whole globe is observed at least once per day, daylight permitting. Besides radiance measurements, the LEO-UVN should make regular observations of the Sun, which are used to compute the Sun-normalized radiance or reflectance, as well as for calibration purposes. It is recommended to make these solar observations at least once per day, to be able to monitor possible changes in the instrument over time.

The spatial resolution follows directly from the user requirements as provided in the MRD. For the UV1 channel a resolution of 50 km (T) / 15 km (G) is recommended. For the UV2, VIS and NIR channels a spatial resolution of 15 km (T) / 5 km (G) is recommended. The spectral bands are defined in Table 4-5. To allow retrieval using a combination of the UV1 and the other channels, it is recommended that the spatial resolution of the UV1 pixel is an integer multiple of the other channels in both the along and the across track direction. The centre of the aggregated UV2/VIS/NIR on the UV1 grid should coincide with the centre of the UV1 pixel.

The spatial resolution as described above is the resolution for which the SNR and other requirements apply. This spatial resolution may be achieved by sampling on a higher resolution and on-ground binning.

Spatial co-registration errors occur for Level 2 products that are based on two or more spectral bands when these observe a different area on the ground. For the LEO-UVN, it is recommended to have a spatial co-registration between the UV2, VIS and NIR bands of 20% (T) / 10% (G).

To provide a quantitatively based recommendation for the spatial response function has proven to be difficult. The requirement in the current MRD of 70% integrated energy in 1 SSD and 90% of the energy in 1.5 SSD seems to be a good requirement. In addition it is recommended to include requirements regarding spatial stray light. Spatial stray light can be defined as light coming from areas outside 3 SSD (TBC). Analyses indicate that pure spatial stray light, e.g. photons from the wrong place on Earth but at the correct wavelengths, is less severe than if it also has a spectral stray light component. The MRD species a spatial stray light scene with bright clouds on either site of a dark scene that is 70 km across track. In the centre of this dark scene the contribution to the reflectance of spatial stray light shall be less than 1%. Tests for ozone and cloud retrievals indicate that the

1% spatial stray light will results in errors of maximum of few percent. For 10% stray light, which may be expected in ground pixels within a few sampling distances from a bright cloud, these errors can be larger than 20%. The test for spatial stray light defined in the MRD is found to be appropriate, although the 70 km for the dark region in the middle of the scene cannot be quantified from simulations. If there is a significant amount of spatial-spectral stray light, the errors can become much larger and should be assessed based on the knowledge of this stray-light contribution, as its effect depends strongly on the exact spectral shape.

The contribution of the spatial stray light should be less than 1% for a dark scene within 3 SSD (TBC) and bright scenes outside this area. For the dark bright scenes the tropical dark and bright reference spectra, as defined in section 4.4.2.4 should be used for he LEO-UVN. For GEO-UVN the reference and maximum reference spectra defined in section 4.4.3.4 should be used.

Due to the Earth curvature and the distance from the instrument to the surface, ground pixels for LEO instruments tend to increase with viewing zenith angle. It is recommended to reduce this effect, for example by reducing the angle over which is integrated in the across track direction for larger viewing zenith angles.

4.4.2.2 Spectral Range

MRD Requirements: MR-LEO-UVN-9

For the LEO-UVN instrument a spectral range from 270 to 500 nm and from 715 to 775 nm is recommended, as illustrated in Figure 4-5. This wavelength range contains all trace gases that can be detected from space in the UV-VIS and includes information on water vapour, cloud and aerosols. SO_2 and formaldehyde will not meet the user requirements for individual measurements (see sections 2.8 and 2.9) and for glyoxal (CHO-CHO), O_2-O_2, BrO, and the aerosol absorbing index (AAI) no user requirements exist in the MRD.

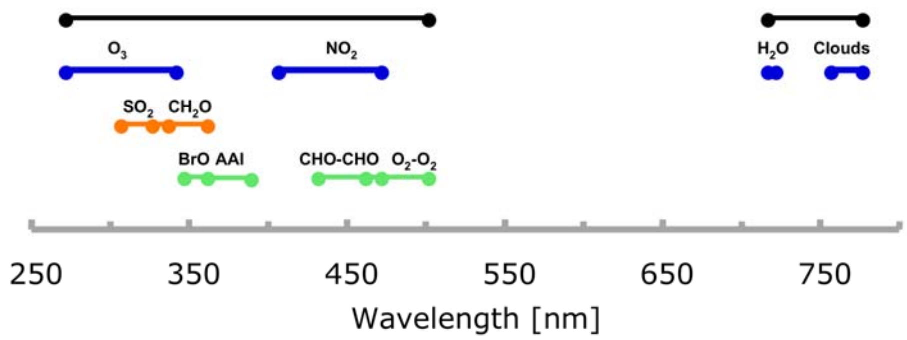


Figure 4-5. Spectral range for the LEO-UVN. Blue lines and symbols are used for species that meet the MRD user requirements, orange is used for species that do not meet the MRD user requirements, and green for species that have no MRD user requirements. The black line and symbols shows the total recommended spectral range.

Due to the different spatial resolution requirements below and above 300 nm, it is recommended to make a band separation in the wavelength range 300-310 nm. From the OMI and GOME experience it is known that such band separation causes problems for ozone profile retrieval, because of the step change in the spectral resolution in combination with the difficulties to establish a consistent radiometric calibration in this region. To avoid such problems as much as possible, it is recommended to make an overlap region between 300 and 310 nm, where the performance is met in both bands. A second logical band separation is in the region 360-380 nm. To be able to derive the absorbing aerosol index from one band, the full performance of the UV2 band should be extended as much as possible to 380 nm. The recommended spectral bands are given in Table 4-5.

4.4.2.3 Spectral Requirements

MRD Requirements: MR-LEO-UVN-10, MR-LEO-UVN-11, MR-LEO-UVN-12, MR-LEO-UVN-13, MR-LEO-UVN-14

The recommended spectral resolution and sampling are given in Table 4-5.
For the NIR band the goal of 0.05 nm spectral resolution is driven by the retrieval of the vertical aerosol profile. The results from this indicate that it is beneficial for this retrieval to have a higher spectral resolution. It is noted that if the spectral resolution is increased, the SNR requirements can be relaxed using the shot noise model and conserving the number of detected photons. In practice the SNR requirements is proportional to the square-root of the spectral sampling.

Table 4-5. Recommended characteristics for the spectral bands for the UVN.

Band	Spectral Range [nm]	FWHM [nm]	Sampling Ratio	SNR[1]	Driving species
UV1	270-310	1.0	3	100 @ 270 nm	O_3
UV2	300-380	0.5	3	1000 @ 310 (320) nm	O_3 (SO_2, CH_2O)
VIS	360-500	0.5	3	1500 @ 420 nm	NO_2
NIR	710-775	0.4 (0.05[2])	3	500 @ 755 nm [4]	Clouds (Aerosols)

1) The SNR is given per spectral sample for a spectral sampling ratio of 3.
2) The goal spectral resolution is driven by the retrieval of the aerosol profile.
3) The start wavelength for the NIR is driven by water vapour; the O_2-A band starts at 755 nm.
4) At higher spectral resolution the SNR may be relaxed. The relaxation can be derived from the shot noise model, assuming that the number of photons on the detector is conserved.

The wavelengths of the spectral channels should be known in-flight with an accuracy of 1/100th of a pixel for the UV2, VIS and NIR bands, and 1/50th of a pixel for the UV1. This knowledge can be obtained in-flight by using the known position of the Fraunhofer lines in the solar spectrum, in combination with knowledge of the slit function. Due to the inhomogeneous filling of the spectrometer slit for inhomogeneous scenes, the centre wavelengths of the spectral channels will vary. To account for this effect, a wavelength calibration has to be performed in flight for each ground pixel. For inhomogeneous scenes the spectral response function will change as compared to homogenous illumination of the instrument. It is recommended to investigate this effect and possible methods in the algorithms to correct for this effect in-flight.

To meet the required knowledge for the spectral calibration, accurate knowledge of the spectral slit function (instrument spectral response function) is essential. The slit function will vary with wavelength as well as with viewing angle. For an accurate description of the slit function $S(\lambda)$, the following information is needed for each spectral sample:

Requirements for the spectral shape of the true in-flight slit function $S_{\mathrm{true}}(\lambda)$ are formulated without prescribing a specific shape model. The slit function is characterized based on pre-flight laboratory measurements e.g. by an analytic function or a spline between tabulated points in dependence of the wavelength and, if applicable, other parameters. The slit function reconstructed from this characterization will be referred to as *modelled* slit function $S_{\mathrm{model}}(\lambda)$.

All slit function requirements refer to the wavelength range Λ, that comprises the main lobe of $S_{\mathrm{true}}(\lambda)$ and that is delimited by the wavelengths where $S_{\mathrm{true}}(\lambda)$ drops below a fraction f_0 = 0.001 (SWIR channel) or f_0 = 0.01 (UV, Vis, NIR channels) of its peak value for the first time with increasing distance from the centre wavelength.

Requirements for the slit function at wavelengths outside the wavelength range Λ are covered by stray light requirements.
The shape of the slit function shall be sufficiently peaked such that the integrated areas satisfy

$$\int_{\mathrm{FWHM}} S_{\mathrm{true}} d\lambda \geq f_1 \int_{\Lambda} S_{\mathrm{true}} d\lambda ,$$

with $f_1 = 0.7$. The integration range on the left side of this equation is the Full Width at Half Maximum (FWHM) of the main lobe of $S_{\mathrm{true}}(\lambda)$; the integration range on the left side is the wavelength range Λ defined in REQ-0.

Spectral features of the true slit function with spectral scales as small as $f_2 = 0.1$ times the FWHM shall be resolved.

The true slit function shall be known with precision errors σ_S that are smaller than $f_{3a} = 0.01$ times the peak value of $S_{\mathrm{true}}(\lambda)$ and smaller than $f_{3b} = 0.1$ times $S_{\mathrm{true}}(\lambda)$ at wavelengths within the wavelength range Λ viz.

$$\sigma_S(\lambda) \leq \min\left[f_{3a} \cdot \max\left(S_{\mathrm{true}}(\lambda)\right), f_{3b} \cdot S_{\mathrm{true}}(\lambda)\right].$$

Deviations of the true in-flight slit function $S_{\mathrm{true}}(\lambda)$ from the modelled slit function $S_{\mathrm{model}}(\lambda)$ shall be smaller than $f_{4a} = 0.01$ times the peak value of $S_{\mathrm{true}}(\lambda)$ and smaller than $f_{4b} = 0.1$ times $S_{\mathrm{true}}(\lambda)$ at wavelengths within the wavelength range Λ viz.

$$\mathrm{abs}\left(S_{\mathrm{true}}(\lambda) - S_{\mathrm{model}}(\lambda)\right) \leq \min\left[f_{4a} \cdot \max\left(S_{\mathrm{true}}(\lambda)\right), f_{4b} \cdot S_{\mathrm{true}}(\lambda)\right].$$

Deviations of the true in-flight slit function $S_{\mathrm{true}}(\lambda)$ from the modelled slit function $S_{\mathrm{model}}(\lambda)$ shall be sufficiently small that the integrated area of the absolute difference is smaller than $f_5 = 0.01$ times the area integrated over the wavelength range Λ viz.

$$\int_{\Lambda} \mathrm{abs}\left(S_{\mathrm{true}}(\lambda) - S_{\mathrm{model}}(\lambda)\right) d\lambda \leq f_5 \int_{\Lambda} S_{\mathrm{true}}(\lambda)\, d\lambda .$$

The width of the slit function expressed as the Full Width at Half Maximum (FWHM) of the main lobe of $S_{\mathrm{true}}(\lambda)$ shall be known accurately with an error smaller than $f_6 = 0.01$ times the true FWHM.

The centre wavelength λ_0 of the slit function, defined by the peak of $S_{\mathrm{true}}(\lambda)$, shall be known accurately with errors below $f_7 = 0.0006$ times the FMHM.

The skewness of the slit function shall be sufficiently small such that the integrated areas in the wavelengths ranges Λ_1 and Λ_2 deviate by less than a factor of $f_8 = 0.66$, viz.

Intra-band spatial co-registration errors occur when different ground scenes are observed for different wavelengths within on band. Intra-band co-registration errors should be better than 20% (T) / 10%(G) for all the spectral bands.

4.4.2.4 Radiometric Requirements

Reference Spectra

MRD Requirements: MR-LEO-UVN-21

For the radiometric requirements the following reference spectra are defined:

- Tropical dark: surface albedo 0.02
- Tropical bright: surface albedo 1.00.
- High-latitude dark: surface albedo 0.02,
- High-latitude bright: surface albedo 1.00.

These tropical spectra are defined for a solar zenith angle of 0 degrees and a satellite viewing angle of 0 degrees, the high latitude spectra for solar zenith angle of 75 degrees. The tropical dark scenario is intended for the definition of the signal-to-noise ratio. The tropical bright and high-latitude dark scenarios are for the dynamical range requirements. For the UV1 the dynamical range is also determined by ozone hole situations (spectrum TBA). The radiance reference spectra are shown in Figure 4-6. The instrument shall not saturate for the signal levels of these reference spectra. In addition, it shall not saturate for ozone hole conditions.

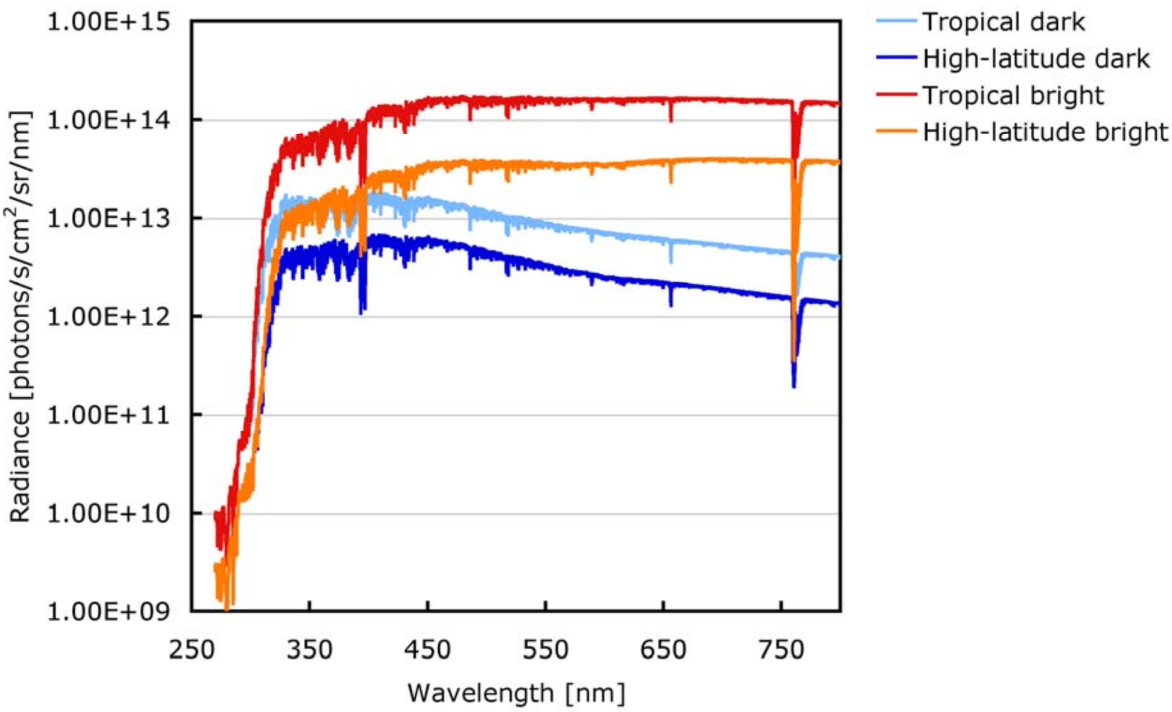


Figure 4-6. Reference spectra for the LEO-UVN. For this plot, a FWHM of 0.3 nm has been used for the complete wavelength range.

Signal-to-noise

MRD Requirements: MR-LEO-UVN-15

The minimum signal-to-noise ratio (SNR) for the radiance in the LEO-UVN bands is specified in Table 4-5, for the tropical dark scenario. In this table the SNR is given at specific wavelengths. The SNR at other wavelengths in a band is obtained by assuming the shot noise model, i.e. that the SNR varies with the square-root of the radiance level. Figure 4-7 shows the SNR values obtained by this procedure for the four wavelength bands. For the conversion to other radiance levels than the tropical-dark reference spectra, it is also assumed that the shot noise model can be adopted.

For the irradiance the SNR should be a factor of ten higher than for the radiance. The reason for this higher signal-to-noise is that one spectrum is used to normalize many radiance spectra. As such, the random noise in the irradiance results in systematic errors for the reflectance. This will cause across track varying errors in the Level 2 products, which can be detected below the noise level of the radiance, due to the systematic nature. The high SNR for the irradiance may be obtained by integrating over a longer time period, because the ground pixel size requirements are not applicable for the solar irradiance.

The threshold signal-to-noise in the UV1 and the UV2 is driven by the ozone profile and ozone column retrieval. For the UV2 band a goal requirement is introduced. This goal requirement will significantly improve the SO_2 and CH_2O retrieval, although not up to the user requirements. The VIS channel SNR is driven by the requirement for boundary layer NO_2. The NIR channel SNR is driven by the requirements for ancillary cloud parameters.

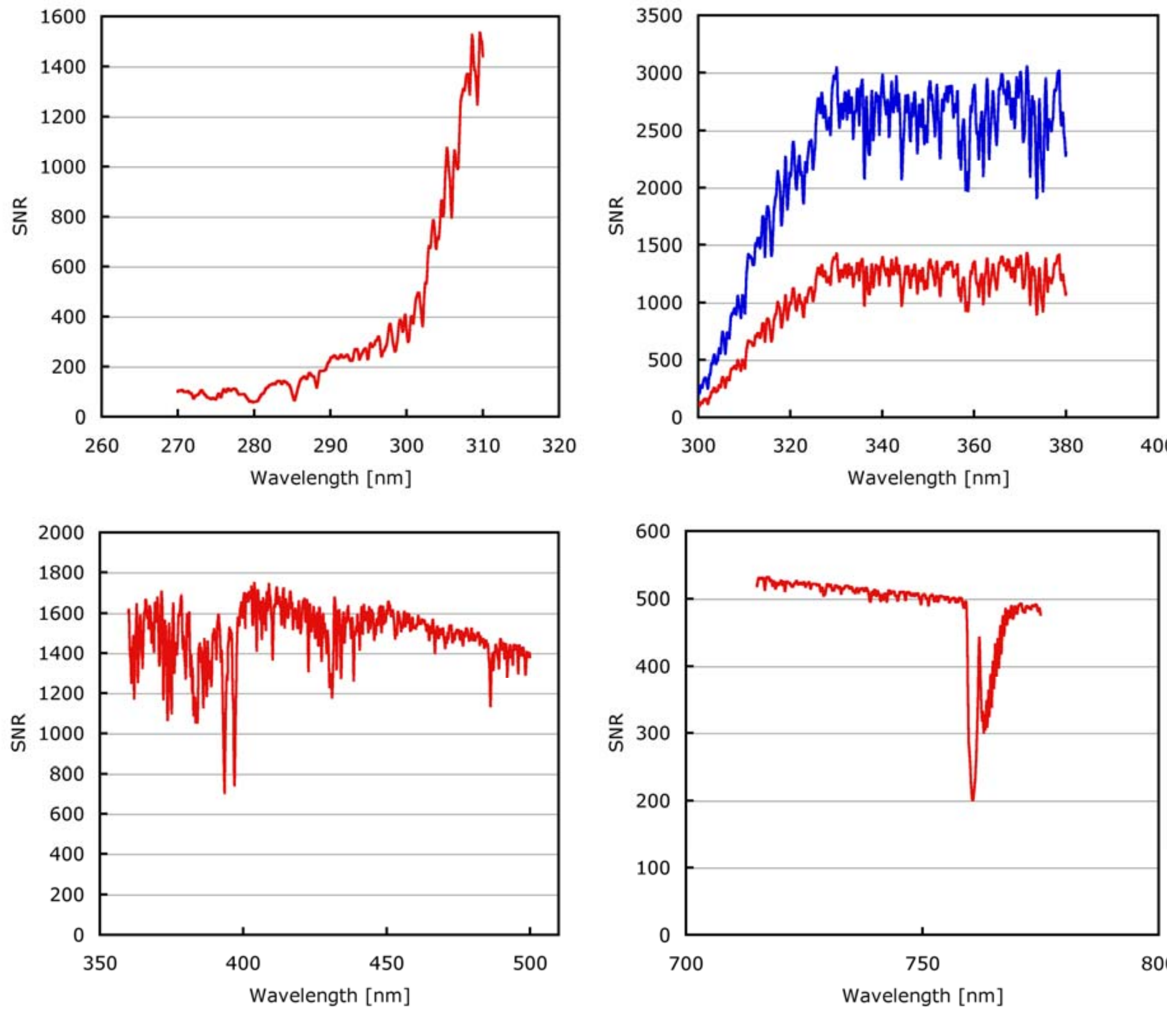


Figure 4-7. SNR for the four bands specified in Table 4-5 for the tropical-dark scenario. For the UV2 a goal (blue) and threshold (red) requirement is specified, for the other bands only a threshold value is used.

Radiometric errors

Multiplicative radiometric errors

MRD Requirements: MR-LEO-UVN-16, MR-LEO-UVN-23

The effect of multiplicative errors on the signal has been modelled using the following equation:

$$I'(\lambda) = (1 + \varepsilon_m)\, I(\lambda),$$

where $I'(\lambda)$ is the perturbed signal (radiance or reflectance), ε_m is the multiplicative error and $I(\lambda)$ is the true signal.

It is recommended to include a requirement on multiplicative errors of 2% (G) and 5% (T) for the reflectance, radiance and irradiance. The goal value of 2% will ensure almost no impact of this type or errors for tropospheric ozone and tropospheric NO_2 for cloud fraction up to 30%. For the threshold value, the impact is within the user requirements.

Additive radiometric errors

MRD Requirements: MR-LEO-UVN-16, MR-LEO-UVN-23

Defining the additive errors is more difficult than for the multiplicative errors, especially for signal with a large dynamical range, e.g. for the radiance in the UV1 and in the NIR. The following equation has been used for the additive errors:

$$I'(\lambda) = I(\lambda) + \varepsilon_a I(\lambda_0),$$

where $I(\lambda_0)$ is the signal at the longest wavelength of a sub-window between λ_0-$d\lambda$ and λ_0 which includes λ.

For ozone profile retrieval in the wavelength range 270 to 330 nm a definition of the additive radiance errors with 5 nm wide sub-windows is used. For the irradiance only one sub-window is used.
For NO_2 six sub-windows are used between 425 and 450 nm for the radiance, and three for the radiance.
For the cloud retrievals one sub-window is used for both radiance and irradiance.

For the UV1, UV2 and VIS bands it is recommended that the additive errors for radiance and irradiance are smaller than 2% (T) and 0.5 (G). For the NIR band the recommended requirement the radiance is 0.1% (T). It should be noted that for the NIR this stringent requirements is due to the dynamical range in the O_2-A band. A 0.1% error in the continuum results in a ~1% error in the deepest part of this band. This result doesn't include possible relaxations by fitting an offset in the retrieval. For the irradiance the recommended requirement for the NIR is the same as for the other bands.

Maximum allowed additive errors in the UV radiance compliant with ozone user requirements depend critically on the definition of the amplitude in the radiance error. In the CAMELOT studies on the cloud impact on UV ozone profile retrieval the additive error amplitude is defined relative to the radiance at a reference wavelength of 300 nm, while the absolute error amplitude is wavelength independent (Figure 4-8). With this definition additive errors are recommended to be smaller than 10% (tropospheric column, boundary column, profile in the free troposphere) or 50% (total column).

An important additive error source is spatial and spectral stray light. The spatially inhomogeneous reference scene for testing for spatial and spatial-spectral straylight has been defined in section 4.4.2.1.

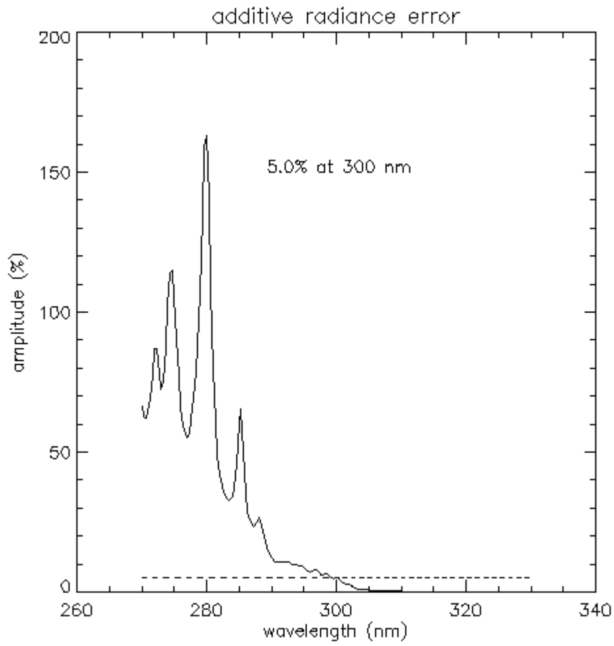


Figure 4-8. Relative amplitude of an additive radiance error of 5%; the amplitude is defined relative to the radiance at 300 nm while the absolute error amplitude is assumed to be wavelength independent.

Relative spatial radiometric errors

MRD Requirements: MR-LEO-UVN-17

The relative radiometric accuracy is a viewing angle dependency with respect to the nadir viewing direction. Such errors can cause viewing angle dependent errors in Level 2 products. It is recommended to keep this requirement at the current value of 0.25%.

Spectral Structures

MRD Requirements: MR-LEO-UVN-18, MR-LEO-UVN-19

Spectral structures are caused by radiometric errors that vary with wavelength. They can cause large errors for retrieval techniques that utilize fine spectral structure, such as DOAS. The errors can be especially large when the spectral structure correlates with one or more gas absorption spectra in the reflectance, as illustrated in Figure 4-9. When this is not the case, the spectral structure may be larger than the recommendation given below. It is strongly recommended to monitor the spectral structures of specific instrument components during the design and build to ensure that they do not interfere wit the trace gases.

For wavelengths in the UV and VIS above 310 nm the spectral structures with a period of 0.1 to ~5 nm in the reflectance should be less than 0.05% (T) or 0.01% (G)[2]. Below 310 nm the requirement can be more relaxed to 0.1% (T). Once the periods and magnitudes of the spectral features are known, the retrieval fit windows should be optimized to minimize the effects of these spectral features.

For spectral structures with periods of 10-100 nm, the radiometric error for the reflectance is covered in the recommended requirements for additive and multiplicative errors given above.

[2] The assessment of the effects of spectral features for the NIR band has not been fully studied in the CAMELOT study. Results for the NIR band are expected as part of the Sentinel 5 Precursor studies.

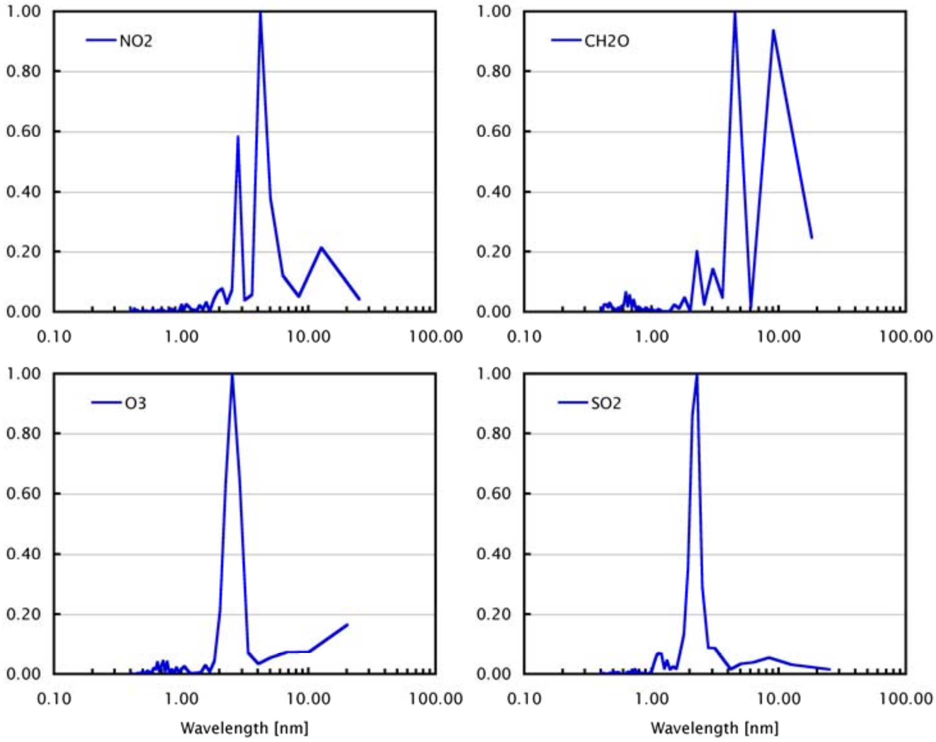


Figure 4-9. Normalized power spectra of the differential absorption spectra of NO_2, formaldehyde, ozone and SO_2. For wavelength periods for which the power spectra peak the retrieval is most sensitive for instrumental spectral features. It is noted that these power spectra depend on the choice of the fit window.

Polarization

MRD Requirements: MR-LEO-UVN-26

Earth radiance can be highly polarised, predominantly due to the Rayleigh scattering. In the UV, the degree of linear polarisation can vary between 0 and close to 1, depending mainly on the Sun-satellite geometry and wavelength. It is recommended to require that the instrument has a maximum polarisation sensitivity of 0.5%.

The effect of errors due to polarization sensitivity should be included in the overall radiometric error budget for multiplicative radiometric errors and for the spectral features.

Solar Irradiance

MRD Requirements: MR-LEO-UVN-23, MR-LEO-UVN-24, MR-LEO-UVN-25

The reference solar spectrum is shown in Figure 4-10. The instrument should measure the solar irradiance without saturating. The solar irradiance measurements are used not only for computing the reflectance, but are also a key measurement to monitor the instrument in-flight. Although this has not been assessed in the CAMELOT simulation, it is recommended to maintain the requirements MR-LEO-UVN-23 and MR-LEO-UVN-24.

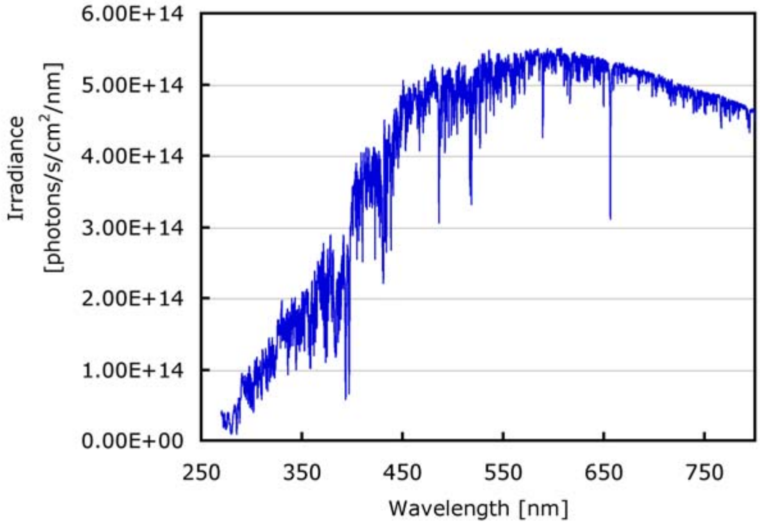


Figure 4-10. Reference solar spectrum calculated for a FWHM of 0.3 nm.

4.4.3 UVN-GEO Requirements

This section describes the requirements for the UVN-GEO instrument. There is a large overlap between the GEO and the LEO instrument, because it aims to measure the same species, but with a limited spatial coverage and with a higher temporal resolution. The temporal resolution follows directly from the user requirements as 0.5 hours (G) and 2 hours (T). An important difference with the LEO-UVN for the UV measurements is that the GEO instrument does not require vertical information on stratospheric ozone, because it focuses on tropospheric ozone.

4.4.3.1 Geometrical and temporal requirements

MRD requirements: MR-GEO-UVN-1, MR-GEO-UVN-2, MR-GEO-UVN-3, MR_GEO_UVN-4

The geometrical requirements for the GEO-UVN are described in the MRD and are derived from the CAPACITY report [http://www.knmi.nl/capacity/]. It is recommended that for the scanning strategy different options are developed that include the following possible scenarios:

- Only scan the areas where the Solar zenith angle less than 90 degrees, this allows for more frequent observations on the east side of the FOV in the morning and at the west side in the evening;
- Less frequent observations over the Atlantic region and more frequent observations over the continent;
- Zoom-in for specific regions to obtain more frequent observation in such a region.

The scan strategy should be developed in close co-operation with the user community.

The spatial resolution requirement following from the user requirements is 15 (T) km / 5 (G) km. Due to the Earth curvature, the pixel size will increase towards the north and towards the east and west of the FOV. It is recommended that these requirements are maintained up to a viewing zenith angle of 70 degrees, which covers the region up to southern Scandinavia, see Figure 4-11.

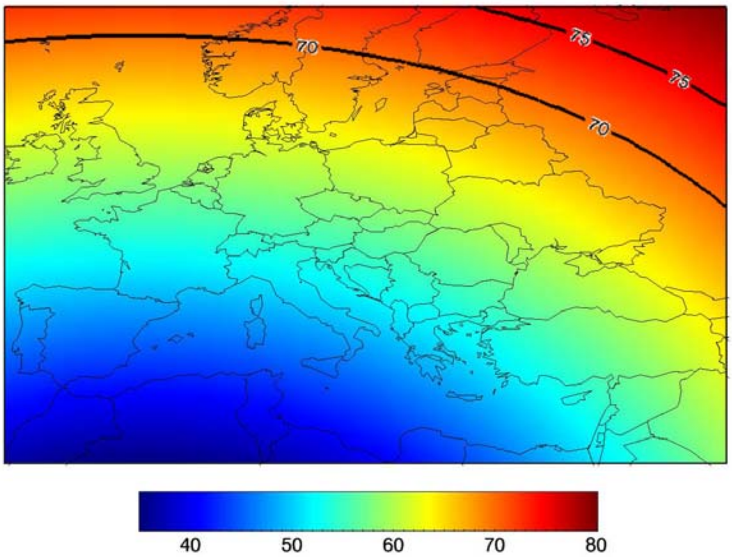


Figure 4-11. Observation zenith angle at the surface for the Sentinel 4 geostationary satellite.

The temporal resolution follows from the user requirements as 0.5 hours (G) / 2 hours (T).

Requirements for the spatial resolution and spatial stray light for the GEO UV, VIS and NIR bands (Table 4-6) are identical as for the LEO UV2, VIS and NIR bands described in section 4.4.2.1. In addition, the requirement on the temporal registration of 15 seconds stated in the MRD seems appropriate.

4.4.3.2 Spectral range

MRD requirements: MR-GEO-UVN-5, MR-GEO-UVN-6, MR-GEO-UVN-7, MR-GEO-UVN-8, MR-GEO-UVN-9, MR-GEO-UVN-10

The spectral range is similar to the LEO-UVN, described in section 4.4.2.2, with the following differences. Because no vertical information in the stratosphere is required, the GEO-UVN can start at 305 nm instead of 270 nm [*Tamminen et al.,* 2009]. If water vapour is assumed to be available from an IR sounder, the NIR channel can start at 750 nm, instead of 710 nm. The recommended spectral bands are given in Table 4-6.

Table 4-6 Recommended characteristics for the spectral bands for the GEO-UVN.

Band	Spectral Range [nm]	FWHM [nm]	Sampling Ratio	SNR[1]	Driving species
UV	305-380	0.5	3	550 @ 310 nm (750 @ 320 nm)	O_3 (SO_2, CH_2O)
VIS	360-500	0.5	3	1500 @ 420 nm	NO_2
NIR	710-775[3]	0.4 (0.05[2])	3	800 @ 755 nm [4]	Clouds (Aerosols)

1) The SNR is given per spectral sample for a spectral sampling ratio of 3.
2) The goal spatial resolution is driven by the retrieval of the aerosol profile.
3) The start wavelength for the NIR is driven by water vapour, the O2-A band starts at 755 nm.
4) At higher spectral resolution the SNR may be relaxed. The relaxation can be derived from the shot noise model, assuming that the number of photons on the detector is conserved.

4.4.3.3 Spectral requirements

All the recommendations given in section 4.4.2 are also applicable for the GEO-UVN, with the following exceptions.

The wavelengths of the spectral channels should be known in-flight with an accuracy of 1/100th of a pixel for all the bands. This knowledge can be obtained in-flight by using the known position of the Fraunhofer lines in the solar spectrum, in combination with knowledge of the slit function.

4.4.3.4 Radiometric requirements

All radiometric requirements described in section 4.4.2 are also applicable for the GEO-UVN, with the following exceptions.

Reference Spectra

MRD Requirements: MR-GEO-UVN-11

Because the GEO-UVN has a limited spatial coverage, the following reference spectra have been specified (see TN-CAM-KNMI-032):

- Reference scenario:
  solar zenith angle 63°, the viewing zenith angle is 57°, surface albedo 0.05 (UV-VIS), 0.15 (NIR);
- Minimum scenario:
  solar zenith angle 80°, the viewing zenith angle is 70°, surface albedo 0.05 (UV-VIS), 0.15 (NIR);
- Maximum scenario:
  solar zenith angle 7°, the viewing zenith angle is 35°, surface albedo 1.1.

The reference scenario is used for assessing the signal-to-noise, the minimum and maximum scenarios are used to assess the dynamical range. The instrument shall not saturate for the signal levels of these reference spectra.

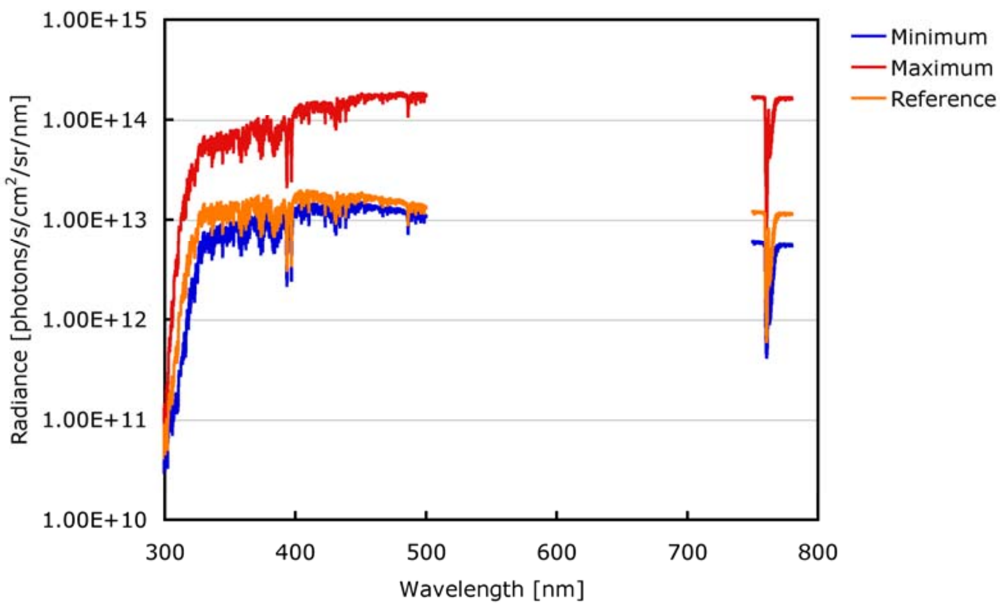


Figure 4-12. Reference spectra for the GEO-UVN. For this plot, a resolution of 0.3 nm has been used for the complete wavelength range.

Signal-to-noise

MRD Requirements: MR-GEO-UVN-11

The recommendations for the GEO-UVN are given Table 4-6 for radiance levels according to the reference spectrum. In this table the SNR is given at specific wavelengths. The SNR at other wavelengths in a band is obtained by assuming the shot noise model, i.e. that the SNR varies with the square-root of the radiance level. Figure 4-5 shows the SNR spectra for all the three GEO bands.
The SNR values are based on the same arguments as for the LEO-UVN. Due to a different choice for the reference spectrum, the SNR values in the tables Table 4-5 and Table 4-6 are different.

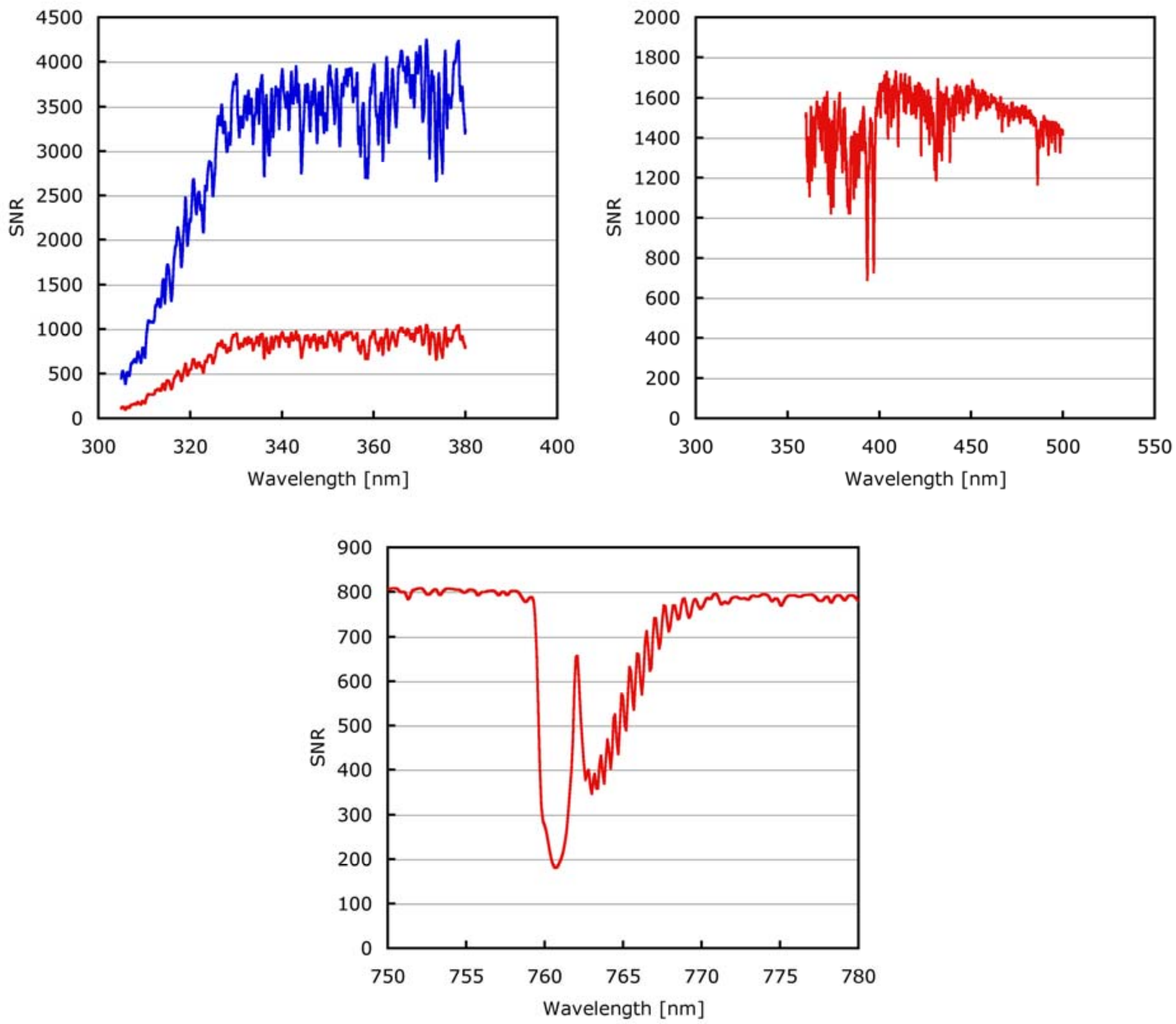


Figure 4-13. SNR for the three bands specified in Table 4-6 for the reference scenario. For the UV band a goal (blue) and threshold (red) requirement is specified, for the other bands only a threshold value is used.

Radiometric errors

Relative spatial radiometric errors

The relative radiometric accuracy is a viewing angle dependency with respect to a reference viewing direction. Such errors can cause viewing angle dependent errors in Level 2 products. It is recommended to keep this requirement on the current value of 0.25%.

Polarization

MRD Requirements: MR-GEO-UVN-23

The Earth radiance can be highly polarised, predominantly due to the Rayleigh scattering. For the GEO Sun-satellite geometry, the degree of linear polarisation can vary between 0 and 0.5, depending mainly on the Sun-satellite geometry and wavelength. It is recommended to require that the instrument has a maximum polarisation sensitivity of 1.0%, when the degree of linear polarisation is varied from 0 to 1.

The effect of errors due to polarization sensitivity should be included in the overall radiometric error budget for multiplicative radiometric errors and for the spectral features.

4.5 Level 1B requirements SWIR

4.5.1 Introduction

In this section the conclusions on the Sentinels 5 the Level 1B requirements are given for the LEO-SWIR instrument. These conclusions are given as recommendations for the MRD Level 1B requirements.

4.5.2 LEO-SWIR Requirements

The SWIR is used to measure the concentration of the trace gases CO, CH_4 and CO_2. In addition the SWIR contains information on the vertical profile of aerosols and clouds and the water vapour column. Within this study, CO and CH_4 are the main drivers for the SWIR channel. Therefore, the Level 1B recommendations described in this section are predominantly derived from the requirements on these gases.

For clear sky scenes SWIR measurements are sensitive to the vertically integrated, total column of CO and CH_4, including the contribution of the tropospheric boundary layer. However, due to the particular light path in the SWIR, the measurements do not have sufficient sensitivity to discriminate any sub-column information. This means that the retrieval of sub column densities depends critically on prior information of the trace gases and thus sub columns are not suited to derive any instrument requirement for the SWIR spectral range. Due to this we decided to derive Level 1B requirements for the 2.3 and 1.6 μm band based on the total column user requirements for CO (25%), CH_4 (2%). With these numbers we set up the total error budget, where we addressed three different error contributions: (1) the retrieval noise, which is the error due to measurement noise, (2) forward model errors, which include errors due to the presence of clouds and aerosols, and (3) retrieval errors caused by errors in the Level 1B product. We assume that nine Level 1B errors occur simultaneously on the measurement. The error budget is summarized in table below:

Table 4-7. Error budget for CO and CH4 used to derive the Level 1B requirements.

Trace gas	Retrieval noise	Forward model error	L1B retrieval bias
CO	11%	8%	3.5%
CH_4	0.6%	1.7%	0.25%

Although different choices of the error budget can be made the error budget reflects our experience with this type of SWIR retrieval.

4.5.2.1 Geometrical Requirements

MRD Requirements: MR-LEO-UVN-1, MR-LEO-UVN-2, MR-LEO-UVN-3, MR-LEO-UVN-4, MR-LEO-UVN-5, MR-LEO-UVN-6, MR-LEO-UVN-7, MR-LEO-UVN-8

The LEO-SWIR instrument should measure the Earth radiance continuously, without gaps in the ground pixels. The instrument should provide daily global coverage, meaning that the whole globe is observed at least once per day, daylight permitting. Besides radiance measurements, the LEO-UVN should make regular observations of the Sun, which are used to compute the Sun-normalized radiance or reflectance, as well as for calibration purposes. It is recommended to make these solar observations at least once per day, to be able to monitor possible changes in the instrument over time.

The retrieval of CO and CH_4 from the SWIR channels will make use of the information on cloud height from the cloud imager and the NIR channel of the LEO-UVN instrument. Given the synergy between these instruments, these should be on the same platform. Assuming that the cloud imager has a much higher spatial resolution as the LEO-SWIR instrument, the co-alignment of these measurements will be achieved, provided sufficient knowledge on the geolocation of the ground pixels. To enable the co-alignment between the NIR channel of the LEO-UVN and LEO-SWIR it is recommended to make the spatial resolution of the LEO-UVN and the LEO-SWIR the same within 20 % (T) and 10% (G) to enable the retrieval of carbon monoxide in partly cloudy conditions. For cloud-free conditions co-alignment should be within 50% of a ground pixel for carbon monoxide retrieval. A possible way of achieving this co-alignment is by measuring the LEO-UVN NIR channel at an integer multiple higher spatial sampling as the LEO-SWIR. On-ground the LEO-NIR channel data that overlap with a LEO-SWIR ground pixel can be re-binned to achieve the best co-alignment.

The retrieval of methane will use both the LEO-SWIR-1 (1.6 μm) and the LEO-SWIR-3 (2.3 μm) bands. Therefore, a co-alignment is needed between these bands of 20% (T). To enable the retrieval of methane in cases of cirrus of aerosol amounts significantly varying on horizontal scales of the order of a few kilometres a 20% (T) co-alignment between the UVN NIR and the LEO-SWIR-1 (1.6 μm) and the LEO-SWIR-3 (2.3 μm) bands is recommended. If the co-alignment errors are larger, the retrieval will be limited to more horizontal homogenous conditions.

4.5.2.2 Spectral Range

Based on the heritage from SCIAMACHY and an analysis of the trace absorption spectra, we recommend a wavelength range of 2305-2385 nm for the 2.3 μm band and of 1590-1675 nm for the 1.6 μm band. One reason for the relatively large spectral ranges is the spectral interference of CH_4, H_2O, and CO in the 2.3 μm band and of CH_4, H_2O, and CO_2 in the 1.6 μm band. The recommended spectral bands are given in Table 4-8.

Table 4-8. Recommended characteristics for the spectral bands for the LEO-SWIR.

Band	Spectral Range [nm]	FWHM [nm]	Sampling Ratio	SNR[1]	Driving species
SWIR-1	1590-1675	≤0.25	2.5 (3.0)	250 in continuum	CH_4 (CO_2)
SWIR-2 [2]	2040-2090	≤0.25	2.5 (3.0)	100 @ 35 10^{12} ph/sr/s/nm 1000 @ 5 10^{11} ph/sr/s/nm	Aerosols
SWIR-3	2305-2385	≤0.25	2.5 (3.0)	100 (120) in continuum	CO, CH_4

1) The SNR is given per spectral sample for a spectral sampling ratio of 2.5.
2) The aerosol height retrievals from the SWIR 2 band are not considered mature. The preferred band for this type of retrieval is the O_2-A band. The numbers for the SWIR 2 channels are estimates based on limited analyses.

4.5.2.3 Spectral Requirements

For both SWIR bands a spectral resolution of 0.25 nm is sufficient. To minimize errors of the spectral interpolation of the solar measurements we propose a sampling ratio of 2.5 (threshold) and 3 (goal).

The required accuracy on the spectral calibration has been analyzed by shifting a simulated reflectance measurement around a nominal wavelength grid. To stay within the error budget of methane a misassignment of larger than 0.002 nm and 0.006 nm must be avoided for the 2.3 μm and 1.6 μm band, respectively. Here any adjustment of the wavelength calibration by the retrieval itself is not considered. For example one can fit a constant wavelength shift of the Earth radiance spectrum simultaneously with other fit parameters of the inversion. Furthermore, a temporary stabile miscalibration of the instrument can be investigated in more depth with a series of consecutive Earth radiance measurements. For example this approach allows one to distinguish between a calibration error and a spectral shift due to an inhomogeneous illumination of the instrument slit. In the latter case the spectral shift varies between consecutive measurements and in addition also affects the shape of the instrument response function. Thus a trade-off has to be made between a strict requirement, which may result in a frequent adjustment of basic instrument properties like the instrument temperature and a stabile instrument performance in time. Taking both aspects into account we recommend to relax the required accuracy and to demand a spectral stability of the Earth radiance measurements between two consecutive solar measurements of 0.005 nm for the 2.3 μm band and 0.012 nm for the 1.6 μm band.

The absorption of CO, CO_2, CH_4 and H_2O in the SWIR shows high spectral dependences, which results in high frequency contributions of the SWIR reflectance spectra. Thus accurate knowledge of the instrument spectral response function (ISRF) is essential. In this study we have investigated the required accuracy for the shape of the instrument response function. For this purpose we simulated reflectance measurements by varying both the FWHM and the shape of the ISRF. For the 2.3 μm band CH4 retrieval simulations have indicated that the FWHM should be known with accuracy better than 1%. For the 1.6 μm band the required accuracy is 0.6%. The shape of the slit function shall agree with a nominal slit function within 1% and 0.7% of its maximum value for the 2.3 μm and 1.6 μm channel, respectively.

4.5.2.4 Radiometric Requirements

To investigate requirements on the radiometric accuracy we distinguished between requirements on the reflectance spectrum and requirements on the earthshine radiance and solar irradiance spectrum. First we investigated the effect of sinusoidal perturbations of the reflectance spectrum on the CO and CH4 retrieval, where we distinguished between an additive and a multiplicative error on the spectrum.

Overall for the 2.3 μm band we found significant CO and CH4 retrieval errors for the sinusoidal perturbations with periods between 0.2 and 100 nm. For sinusoidal additive and multiplicative errors with periods 0.2-100 nm the error shall at most 0.15% (3σ) for the threshold and 0.07% (3σ) for the goal performance of the instrument. Additionally, the CH4 retrieval is sensitive to an additive wavelength independent offset of the reflectance measurement, which shall not exceed 0.1%. Multiplicative wavelength independent errors can be compensated to a large extent by the fit of a wavelength independent surface albedo. However in presence of cirrus this error shall not exceed 1.5%.

For the 1.6 μm band additive errors with periods of 0.2-300 nm shall be at most 0.06% (3σ) for the threshold and 0.03% (3σ) for the goal performance of the instrument. Multiplicative errors of the same period domain shall be at most 0.08% (3σ) for the threshold and 0.04% (3σ) for the goal performance of the instrument. Multiplicative wavelength independent errors shall not exceed 2% whereas wavelength independent offset shall not exceed 0.1%.

Overall, a sinusoidal spectral perturbation may not reflect a realistic Level 1B radiance error and in practice a superposition of different periods may occur. This can lead to larger error propagation but could also cause smaller propagation of error. Thus we recommend monitoring the effect of spectral features during the design and build of the instrument.

Requirements on the absolute accuracy of the earthshine radiance and solar irradiance measurements cannot be derived from retrieval simulations, which are based on the reflectance spectrum only. However, experience with existing instrument has shown that the earthshine radiance and solar irradiance measurements provide useful information on the instrument performance. Based on these experiences we propose an accuracy of 2% on the earthshine radiance and solar irradiance measurements for both the 1.6 and 2.3 μm band.

To study spatial stray light we consider two scenes where one scene is cloud-free and the other scene contains a cloud layer at high altitude. If a measurement, which points to the centre of the clear sky scene, is also sensitive to the cloudy scene then the measurement is subject to spatial stray light. Generally both scenes do not have to be adjacent ground pixels but the clear sky pixel can also be embedded in a larger cloud-free neighbourhood. However, to exploit as much as possible cloud-free observations it is obvious to formulate the requirements for scenes with smallest spatial distance. To simplify matters we assume that spatial stray light causes an additive error and so requirements on stray light are already covered by the radiometric requirements. Due to its importance for the instrument performance they are mentioned as an extra requirement. Here we propose that an additive wavelength dependent contribution of stray light to the reflectance spectrum of a dark scene shall be smaller than 0.15% (3σ) for the 2.3 μm band and smaller than 0.06% (3σ) for the 1.6 μm band. An additive wavelength independent stray light contribution shall be smaller than 0.1% for both spectral bands. It is important to realize that the solar geometry shall be the same for the dark and bright scene.

In the SWIR light gets polarized mainly by reflection at vegetation surfaces. Here the reflected light can have a degree of linear polarization of up to 0.4 in both spectral bands, depending on the scattering geometry at the surface. The effect of aerosols is less relevant in this context. The degree of linear polarization shows only very little spectral features that are caused atmospheric scattering and absorption. Although these features interfere inherently with absorption structures they can be ignored in the retrieval for polarization sensitivities between -0.2 and 0.2 for both SWIR channels. Problems may occur when spectral features of the polarization sensitivity are similar to trace gas absorption structures. To avoid this we propose that the amplitude of spectral features in the polarization sensitivity with periods < 300nm shall not exceed 0.01 (3σ). The polarization sensitivity with periods >300 nm shall be known with an absolute accuracy better than 0.04.

4.6 Level 1B requirements TIR

4.6.1 Introduction

Requirements for the TIR sounder in the previous versions of the Sentinels 4-5 MRD –up to version 2.0 from August 2008– were set considering a few target species, with the additional objective to provide a subset of narrow spectral ranges for each. The spectral ranges included some bands (e.g. LEO-TIR-1) without clear-cut demonstration of the possibility to retrieve the products. For the GEO-TIR only three bands, targeting O_3, CO and HNO_3 were initially kept.

During the project, the decision to the merge Sentinel 4-5 and Post-EPS and MTG programmes has significantly changed the perspective. In particular, the GEO-TIR component of the system concept for Sentinel 4 was abandoned due to partial overlap with the MTG-IRS instrument design at EUMETSAT. The latter is not being optimized for chemistry/air quality applications and so, the relevance of the CAMELOT study for the GEO-TIR component is out of scope and will not be considered here [*]. The LEO-TIR system concept was fully studied for integration on Sentinel 5. Strongly revised recommendations in comparison with MRD version 2.0 are provided hereafter, on the following grounds:

- *Results from CAMELOT sensitivity studies* to TIR Level 1B requirements for O_3, CO, CH_4, HNO_3 and PAN as well as for H_2O.
- *IASI lessons*. These refer principally to the capabilities of the sounder for monitoring tropospheric composition under various conditions (e.g. surface type, thermal contrast), including for measurements of short-lived species never probed before from space, from local (source identification) to global (transport and chemistry) scales.
- *Homogenisation between Sentinel 5 and Post-EPS MRD*

[*] We refer to http://www.EUMETSAT.int/groups/pps/documents/document/pdf_mtg_rep38.pdf for a detailed description of MTG-IRS specifications and for an overview of the potential of this instrument to contribute to atmospheric pollution monitoring in comparison to a S4 type of instruments

4.6.2 LEO-TIR Requirements

4.6.2.1 Geometrical Requirements

MRD Requirements: MR-LEO-TIR-1, MR-LEO-TIR-2, MR-LEO-TIR-3, MR-LEO-TIR-4, MR-LEO-TIR-5, MR-LEO-TIR-6, MR-LEO-TIR-7, MR-LEO-TIR-8

The LEO-TIR instrument should measure the Earth radiance continuously, ideally without gaps in the ground pixels. The TIR sounder here will make observations in the nadir geometry and off-nadir using the Earth and atmospheric thermal emission as a source. As it is not relying on solar radiation, data shall be acquired continuously during day and night time. The IRS shall provide 90% global coverage within 12 hours and 100% within 24 hours. Spatial and temporal sampling should be given high priority.

The spatial resolution follows directly from the user requirements as provided in the MRD. A spatial resolution of 12 km (T) / 5 km (G) is recommended. The geolocation accuracy shall be known to better than 5 km (threshold), 500 m (goal).

MR-LEO-TIR-1. Data acquisition shall be performed continuously at nadir and perpendicular to the flight direction
MR-LEO-TIR-2. The instrument shall maximise the useful viewing angle and provide 90% global coverage within 12 hours and 100% within 24 hours
MR-LEO-TIR-3. The spatial resolution at SSP shall be 12 by 12 km^2 (T) / 5 by 5 km^2 (G).
MR-LEO-TIR-4. The off-nadir spatial resolution shall be obtained by maintaining the same solid angle of the FOV.
MR-LEO-TIR-5. The IE over a squared area (resp. circle) covered by the spatial resolution shall be larger than 90%.
MR-LEO-TIR-6. The IPSF shall be flat to within 5% peak-to-average within a diameter of 80% of the spatial resolution.
MR-LEO-TIR-7. The IPSF shall be characterised within a diameter of 200% of the spatial resolution.
MR-LEO-TIR-8. Deleted

4.6.2.2 Spectral Requirements

MRD Requirements: MR-LEO-TIR-9, MR-LEO-TIR-10, MR-LEO-TIR-11, MR-LEO-TIR-11, MR-LEO-TIR-12, MR-LEO-TIR-13

Spectral range (MR-LEO-TIR-9)

The requirements for spectral range have been extensively revised following CAMELOT recommendations but also considering the IASI experience for monitoring short-lived species of relevance for atmospheric chemistry and indirectly air quality and climate. The priorities for the species included in early versions of the MRD have been mainly unchanged while proposition of priorities are given for the species that were not considered to now. This range of priorities has been formulated according to species and application (See Table 5-1). For example, O_3 and CO are considered important air quality species and are given priority 1. Whereas, SO_2 in the boundary layer is hardly traceable in the TIR spectral range and is given a priority 2.

MR-LEO-TIR-9: The TIR sounder shall cover the spectral bands according to the ranges as specified in Figure 4-14 taking into account the priorities and optional alternative bands. Extended wavenumber coverage is strongly preferred over narrower independent windows, as it allows numerous species and aerosol to be probed simultaneously (Figure 4-14). Especially the 700-1400 cm^{-1} spectral range shall be covered without gaps, with additional coverage between 2000-2200 cm^{-1} (narrowing possible) and 2700-2900 cm^{-1} (TBC)

Table 4-9. Spectral requirements and NeDT values for TIR LEO sounder. G, B and T refer to Goal Breakthrough and Threshold values.

Band	Application[a]	Spectral range (cm^{-1})[a]	Species	Priority	Spectral resolution (cm^{-1}) G/B/T	NeDT (K @ 280K) G/B/T
					Unapodised	Unapodised
1	AC	650-750	C_2H_2, HCN	3	0.15/0.225/0.30	0.07/0.14/0.25
2	AC	750-850	PAN (H_2O, HONO, C_2H_6, NH_3, CFC11)	2	0.15/0.225/0.30	0.07/0.14/0.25
3	AC	850-920	HNO_3 (H_2O, NH_3, CFC11)	1	0.075/0.15/0.30	0.07/0.14/0.25
4	AC, AQ	920-980	NH_3, C_2H_4 (CFC12)	1	0.075/0.15/0.30	0.07/0.14/0.25
5	AC, AQ, C, OP	980-1080	O_3, CH_3OH (NH_3)	1	0.075/0.15/0.30	0.07/0.14/0.25
6	AC, C	1080-1130	HCOOH (SO_2, NH_3, CFC12)	2	0.15/0.225/0.30	0.07/0.14/0.25
7	AC, AQ	1130-1200	SO_2 PBL-FT (PAN, NH_3, CFC12)	3	0.15/0.225/0.30	0.07/0.14/0.25
8	AC, C	1200-1350	CH_4, H_2O[b] (N_2O, HNO_3, SO_2-UT)	2	0.15/0.225/0.30	0.07/0.14/0.25
9	AC	1350-1400	SO_2-UT[c] (H_2O)	2[c]	0.15/0.225/0.30	0.07/0.14/0.25
10	AQ, OP, AC	2050-2250	CO	1	0.075/0.15/0.30	0.07/0.14/0.25
11	AC, C	2700-2900	CH_4	3	0.15/0.225/0.30	0.14/0.25/0.3

a) *AC: Atmospheric Composition, AQ: Air Quality; C: Climate; OP: Operational application*
b) *Includes suitable information for heavier water isotopologues. Note that for water vapour the requirements are met only by combining the dedicated band with the 800-900 cm^{-1} interval (bands B2+B3), which is more sensitive to the surface content.*
c) *Priority 2 justified by demonstrated operational aerial safety applications*

Spectral resolution (MR-LEO-TIR-10)

TIR instruments with a range of spectral resolutions have been and are still operating. These instruments provide sensitivity to tropospheric composition but vary in vertical resolution and in the degree of sensitivity to the surface. As clearly assessed during this study, higher spectral resolution leads to improvements for both aspects and should be pursued as much as possible to approach Level 2 requirements on target species. For some species, high spectral resolution (below or equal to breakthrough levels in Table 4-9) is needed to decorrelate stratospheric and tropospheric sub columns. Overall however, target error requirements on the integrated tropospheric columns are achieved for most species even at medium resolution (IASI-like instrument), which is considered here to be threshold resolution.

Note: The threshold is to be understood as “the minimum performance below which the data would have no value in supporting identified operational applications”. The threshold requirements for spectral resolution and radiometric noise are those, or closely approach those, of IASI, which has demonstrated performances for monitoring atmospheric chemistry and for supporting operational applications. These medium resolution, threshold requirements will not allow reaching some of the most stringent Level 2 requirements defined for Sentinel 5 operation, namely the vertical resolution in the troposphere and the improved sensitivity to the surface. To improve upon these products, goal and breakthrough requirements should be pursued.

<u>MR-LEO-TIR-10a</u>: The unapodised spectral resolution shall be within the range of goal-threshold values specified in Table 4-9. Unapodised spectral resolution has to be understood as $\Delta\tilde{\nu}_{na} = \frac{0.6}{OPD_{max}}$ *for a Fourier*

Transform spectrometer (thus the IASI-like unapodised spectral resolution is 0.3 cm^{-1}). This corresponds to the FWHM of the sinc(x) function.

MR-LEO-TIR-10b: In the case of a Fourier Transform Spectrometer, the self-apodisation effect shall be minimised. The FWHM of the instrument line shape (including self-apodisation but excluding any apodisation function applied in post-processing of the data) for any spatial resolution element within the FOV shall not exceed the unapodised spectral resolution by a factor larger than about 1.4 (to be confirmed) throughout the measured spectral range, excluding band 11.

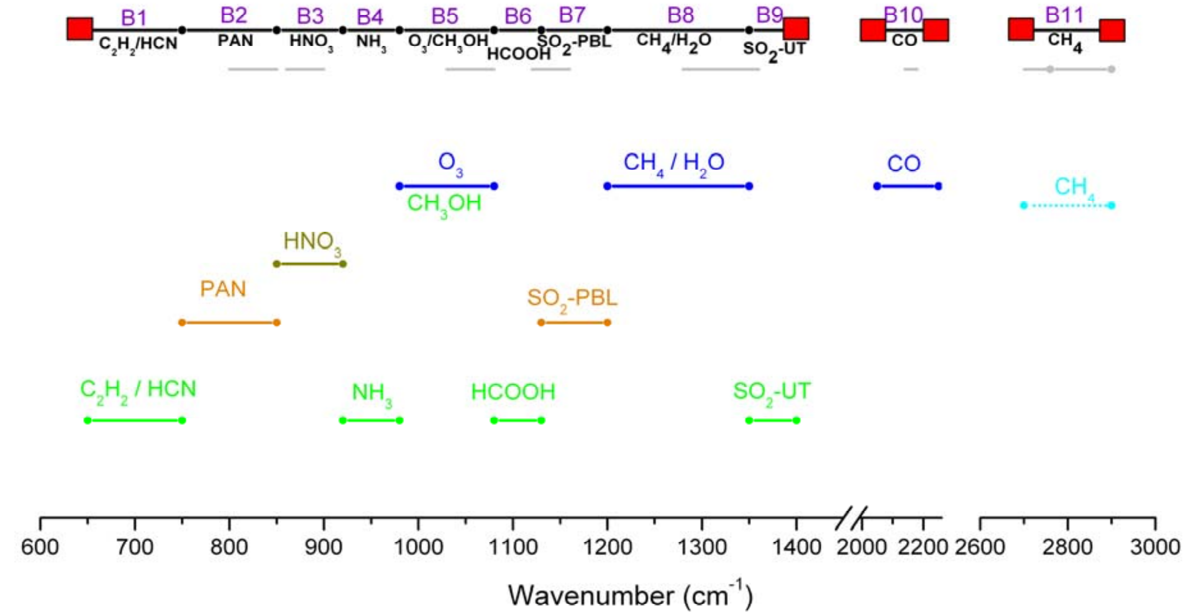


Figure 4-14. Spectral range for the LEO-TIR. Blue lines and symbols are used for species that meet most of the MRD user requirements, orange is used for species that do not meet the MRD user requirements, and green for species that have no MRD user requirements. Dark yellow is used for HNO_3, which meets some user requirements and cyan for the shortwave end, which has not been tested here. The black line and symbols shows the total recommended spectral range (numbered from B1 to B11), with the red squares the upper and lower bounds in between which continuous coverage is targeted. The light grey lines show the spectral ranges from MRD-v2.0. Note that for water vapour the requirements are only met by combining the dedicated band with the 800-900 cm^{-1} interval (bands B2+B3), where the latter is more sensitive to the surface content.

Spectral sampling (MR-LEO-TIR-11)

MR-LEO-TIR-12: The spectral sampling shall be 0.5 / OPD_{max}

Spectral calibration (MR-LEO-TIR-12, MR-LEO-TIR-13)

MR-LEO-TIR-12: For a spatially homogeneous scene, the Instrument Response Function of each spectral sample shall be known with an accuracy satisfying:

$$\int_{\mathfrak{D}} \left|\Delta ISRF(\tilde{\nu})\right| \partial\tilde{\nu} \le 0.02$$

$$\int_{\mathfrak{D}} ISRF(\tilde{\nu}) \partial\tilde{\nu} = 1$$

with $\mathfrak{D}$ the interval of $\tilde{\nu}$ where $\frac{\left\|cISRF(\tilde{\nu})\right\|_2}{\left\|cISRF(0)\right\|} \ll \frac{1}{SNR}$

MR-LEO-TIR-13: The position of the spectral samples centres shall be known with an accuracy better than a tenth of the spectral sampling: $\delta\tilde{v} < \frac{1}{10}\left(\frac{0.5}{OPD_{\max}}\right)$

4.6.2.3 Radiometric Requirements

MRD Requirements: MR-LEO-TIR-14, MR-LEO-TIR-15, MR-LEO-TIR-16, MR-LEO-TIR-17, MR-LEO-TIR-18, MR-LEO-TIR-19

Notes:

- The NeDT values are specified with a reference blackbody at 280 K.
- Additive errors apply linearly in brightness temperature following $\alpha^{add}(K) = \left|BT^{ref}(\tilde{v}) - BT(\tilde{v})\right|$, where BT^{ref} is the brightness temperature from the unperturbed scene, as obtained by inverting the blackbody function, and BT is the perturbed brightness temperature, offset by a factor α^{add} as compared to BT^{ref}.
- Multiplicative errors apply on the radiances: $L^{'}(\tilde{v}) = \alpha^{mult} \cdot L(\tilde{v}) + L(\tilde{v})$.

Radiometric noise (MR-LEO-TIR-14)

MR-LEO-TIR-14: The NeDT values shall be within the range goal to threshold values (unapodised) as specified in Table 4-9.

MR-LEO-TIR-14b: The apodised noise values are expected to be smaller than the unapodised noise values by a factor 1.4-1.7.

Radiometric accuracy (MR-LEO-TIR-15)

MR-LEO-TIR-15: The absolute radiometric accuracy shall be better than 0.5 K for a reference brightness temperature TOA at 280 K.

Radiometric stability (MR-LEO-TIR-17)

MR-LEO-TIR-15: The data acquired in each spectral channel shall be constant to within at least 0.1 K (T) / 0.05 K (G) over one orbital period, assuming a stable and spatially uniform scene of 280 K TOA brightness temperature.

Relative radiometric accuracy (MR-LEO-TIR-17, MR-LEO-TIR-18)

MR-LEO-TIR-17: The relative spectral radiometric accuracy over the complete spectral range within a TIR band shall be smaller than 0.2% RMS (0.11 K at 1000 cm^{-1}) assuming a stable and spatially uniform scene of 280 K TOA brightness temperature.

MR-LEO-TIR-18: The relative spatial radiometric accuracy over the complete spectral range within a TIR band shall be smaller than 0.2% RMS (0.11 K at 1000 cm^{-1}) assuming a stable and spatially uniform scene of 280 K TOA brightness temperature.

Dynamic range (MR-LEO-TIR-19)

MR-LEO-TIR-19: The dynamic range of the TIR sounder shall be optimized to cover the spectral radiances for nadir measurement scenes ranging from clear-sky hot desert (330 K) to cold icy locations (180 K).

An example of a radiance / brightness temperature spectra for a scene at 295 K is provided in Figure 4-15.

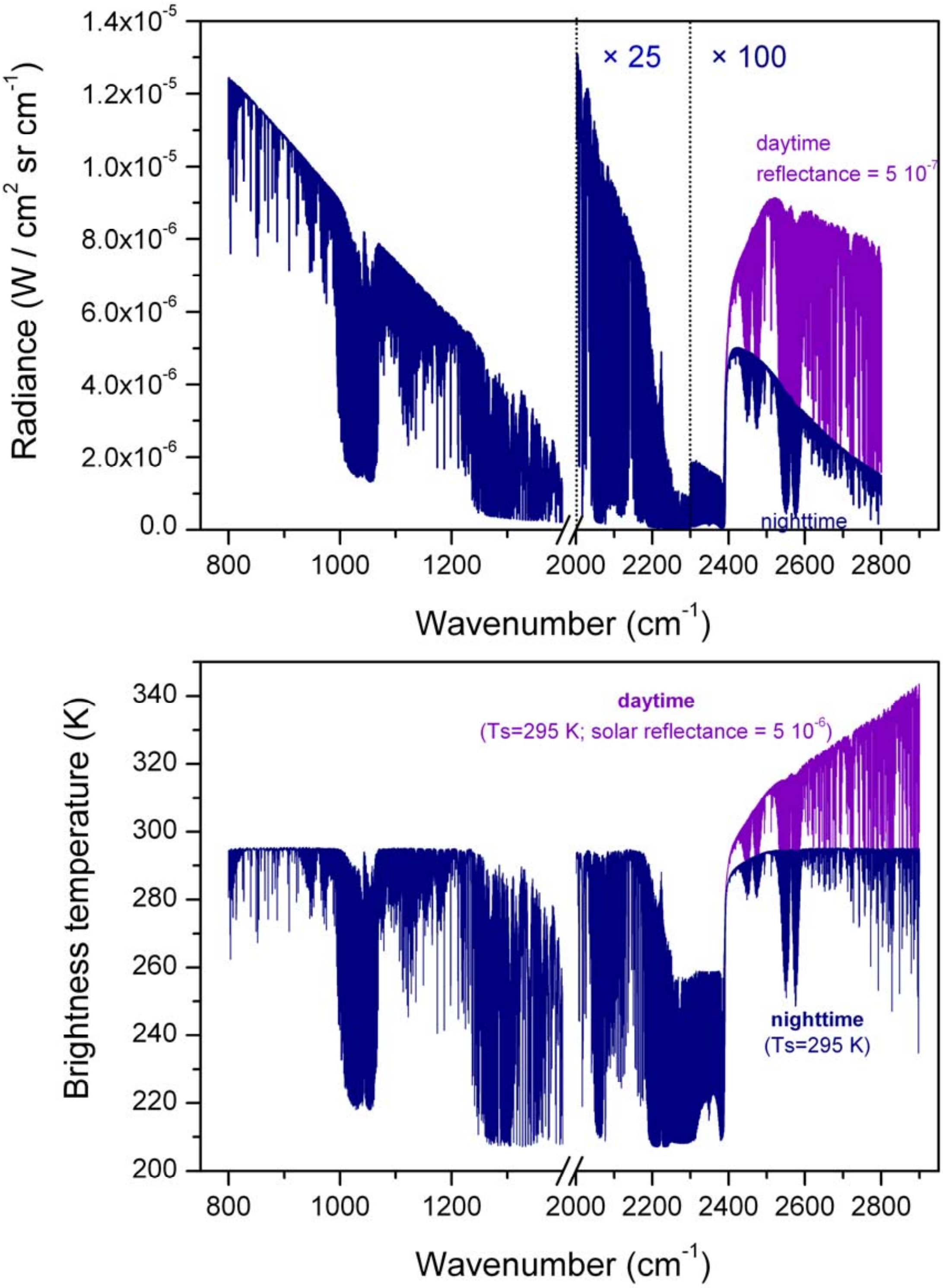


Figure 4-15. Example of radiance (top) and corresponding brightness temperature spectra (bottom) for a uniform reference scene at 295 K and unitary emissivity, simulated without instrument response function. The purple spectrum is a daytime simulation assuming an effective surface reflectivity of $5x10^{-7}$.

4.6.3 TIR-GEO Requirements

We refer to http://www.EUMETSAT.int/groups/pps/documents/document/pdf_mtg_mrd.pdf for the current status of MTG-IRS specifications and to http://www.EUMETSAT.int/groups/pps/documents/document/pdf_mtg_rep38.pdf for a comparative analysis of its expected performances for chemistry /air quality applications.

4.7 Level 1B requirements DPI

The primary aim of the Directional and Polarization Imager (DPI) is to provide information on aerosol optical properties (optical thickness, single scattering albedo) and microphysical properties (size distribution, refractive index) with sufficient accuracy for climate and air quality applications. DPI will also provide information on cloud properties and surface Bi-Directional Reflection Function (BDRF). The Level 1B requirements given below are based on retrieval simulations performed within the ESA CAMELOT study, together with a review of the 3MI Level 1B requirements given in the EUMETSAT Post-EPS Mission Requirement document. The Level 1B requirements are based on Level 2 user requirements formulated by Mishchenko et al. (2004) for the Advanced Polarimetric Sounder (APS) on the NASA-GLORY mission. It should be noted that the 3MI requirements that refer to a specific instrument concept (based on POLDER) are not considered here, since it is not clear if the required polarization accuracies can be achieved with such an instrument concept.

4.7.1 Spectral Requirements

MRD_3MI.020
The DPI should measure total reflectance and Stokes fractions q = Q/I and u = U/I at multiple viewing angles (at least 10) in the spectral channels listed in Table 4-10 with polarization in a subset of these spectral channels.

Table 4-10. Wavelength, FWHM and polarization specification for channels of the DPI.

Channel	Central wavelength (nm)	FWHM (nm)	Polarization
1	354	20	N
2	388	20	Y
3	443	20	Y
4	490	20	N
5	555	20	Y
6	670	20	Y
7	745	20	N
8	865	40	Y
9	1370	40	Y
10	1650	40	Y
11	2130	40	Y

These spectral bands capture the typical spectral dependence of aerosols, allow for surface characterization in the shortwave infrared (band 10) where the aerosol contribution is mostly small, and allow for cirrus characterization from band 8 with strong water vapour absorption (meaning that all signal measured originates from scattering above the bulk of the water vapour). Compared to the 3MI MRD some small changes are made: 1) Band 3MI-1 (342 nm) is left out because simulations have shown that this band does not significantly improve the accuracy on the aerosol properties while it is demanding to realize from an instrument point of view. 2) The bands 3MI-7 and 3MI-8 around the O_2-A band are left out because at this spectral resolution only very limited information on cloud height can be retrieved. Independent cloud height from a TIR imager should be preferred (not affected by aerosol scattering). Instead of bands 3MI-7 and 3MI-8, channel 6 is placed at 745 nm, to minimize the effect of gas absorption. 3) Channel 8 (3MI-10) also needs to measure polarization because the retrieved cirrus properties from this channel are used to describe total reflectance as well as polarization in the other channels for aerosol retrievals under thin cirrus conditions.

MRD_3MI.100
The spectral response of the channels shall be known, with 0.5 nm sampling, to 1% of their peak response at any wavelength (TBC).

MRD_3MI.150
The spectral response stability shall be less than 0.1 nm (TBC).

4.7.2 Radiometric Requirements

MRD_3MI.210
The radiometric noise shall be better than
sup [0.0005, 0.005R] for total reflectance channels.
sup [0.001,0.01R_p] for all polarized channels.

Although the simulations reported in the CAMELOT Task 3 report are performed with a different noise specification (SNR = 1000 for a Lambertian equivalent reflector with albedo of 0.40), it is confirmed by new simulations for a subset of the scenarios that the noise values specified above (the 3MI specifications) are also sufficient to meet the user requirements.

MRD_3MI.300 / MRD_320
The radiometric calibration error should be better than 1% (goal) – 4% (threshold) for the total reflectance and the inter calibration error between nadir and fore/aft viewing directions shall be < 1%. The latter requirement is more strict than the 2% in the 3MI MRD, because an inter-calibration error of 2% between nadir and fore/aft viewing can result in an AOT error of 0.06, well above the user requirement.

The radiometric calibration error on Stokes fractions q and u should be smaller than 0.002 (goal) and 0.005 (threshold). A requirement on q and u is not included in the 3MI MRD but the accuracies given above are essential to meet the user requirements on single scattering albedo and refractive index. It should be noted that the POLDER instruments achieves an accuracy on q and u of 0.01-0.02, which should be significantly improved.

4.7.3 Geometric Requirements

MRD_3MI.630
A ground pixel should be observed (almost) simultaneously under at least 10 viewing angles in the range -50^{o} to 50^{o}. Simulations point out [Hasekamp and Landgraf, 2007] that measurements at five viewing angles (equally spread between fore and aft views) are already sufficient for aerosol retrievals. However, measurements at some viewing angles may not be usable due to glint or cloud contamination. Therefore, measurements at more viewing angles should be available and we adopt the 3MI specification here.
Acquisition of measurements close to the principal plane should be maximized. Simulations point out that the requirements on the relevant aerosol parameters are met under most circumstances for relative azimuth angles < 40^{o} (defined such that a relative azimuth angle of 0^{o} corresponds to the principal plane).

MRD_3MI.640
The on ground pixel size shall be less than 1 km (goal) – 2 km (threshold)

MRD_3MI.700 – MRD_3MI.720
The spatial co-registration between polarized components and different viewing angles shall be less than 10% of the pixel diameter. The spatial co-registration between different spectral channels shall be less than 20% of the pixel diameter. It should be noted that it is extremely difficult to check these numbers, as this would require information about surface reflectance on spatial scales smaller than 100 m.

4.7.4 Auxiliary Requirements

Retrievals from the DPI should be supported by measurements of cloud height in the thermal infrared (TIR) spectral range. This information is essential for cloud screening and may be used to perform simultaneous retrievals of aerosol and cloud properties for scenes with an elevated aerosol layer above the cloud top, and for partly clouded pixels with small cloud fractions.

5 Assessment of Cloud Contamination

5.1 Integrated approach to Task 4 and 5

The aim of Task 5 "Optimisation of orbit scenarios" is to quantitatively assess the sampling characteristics of particular orbit scenarios for particular level 2 products. This assessment needs to connect the sensitivity of each level 2 product to various parameters, including cloud, to the sampling of these parameters encountered by a particular orbit type, as a function of location and time.

Task 4 has supports this assessment by providing statistics on the occurrence cloud within the field-of-view (FOV) of Sentinel 4/5 sensors, as a function of

- geographical region
- season and time of day,
- pixel size and observation geometry

Task 5 then combines the retrieval sensitivities of particular level 2 (L2) products to cloud and observing conditions with the cloud occurrence to infer spatio/temporal sampling of retrievals compliant with user-requirements. On that basis the benefits of various mission options are then assessed.

In approaching task 4 and 5, the following observations were made:

- The assessment in Task-4 (and hence -5) relies on the existence of an extensive dataset of cloud properties. Several data sets exist e.g., however no single data set is perfectly suited to the purposes of this study. Since a key objective is to trade-off the relative benefits of geostationary (GEO) vs. low earth orbit (LEO) and to optimise the local time(s) of LEO, cloud statistics have to be based on a geostationary cloud data-set.
- Such a data set provides the only basis to derive cloud statistics (within the observed disk) which are representative of both LEO and GEO orbit (albeit with limitations with respect to LEO which are addressed by cross-referencing to MODIS cloud statistics).
- To draw meaningful comparative conclusions for GEO and LEO, the only reliable approach is to use a single cloud data set as a common basis from which to synthesize all the different orbit configurations. If instead data sets were to be derived from different sensors (e.g. one LEO and one GEO) were to be used, this would seriously compromise the validity of the comparison, and therefore the conclusions, due to significant differences between cloud analyses from different instruments.
- To allow the logical flow from retrieval sensitivity via cloud occurrence to assessment of orbit configurations, it is essential that retrieval sensitivity to cloud parameters is quantified in terms of the same cloud variables as the geostationary cloud data-set to be used to generate the statistics.
- The most important criterion to the Sentinel applications to be considered in this study is whether or not the boundary layer is visible, and cloud at virtually any altitude will obscure the boundary layer. Cloud height is therefore somewhat less critical (compared to cloud fraction and opacity) to the main focus of this study.
- Both retrieval sensitivity and cloud occurrence depend on a number of variables which co-vary along any given orbit. It is not considered practical (or useful) to generate cloud statistics which comprehensively span this multi-variate data-space. Instead the approach adopted is as follows:
    - In Task 4, a reference set of basic statistics on the likelihood of cloud-free scenes is generated and the sensitivity to levels of cloud-contamination (fraction, opacity, height) assessed.
    - In Task 5, statistics on the likelihood of good L2 retrievals are generated directly by applying an operator (specific to each retrieval product) to the cloud-dataset at full temporal and spatial sampling. In essence, for each product the responsible retrieval team populates a multi-dimensional look-up-table (LUT) which defines the region in which a retrieval meets user requirements, as a function of the cloud parameters which affect retrieval sensitivity (i.e. fraction, opacity and height). This LUT is then "flown" through the cloud-dataset and for each individual observation (integration period/ field of view) the correct parameters for the orbit are determined and the LUT used to determine whether or not the retrieval is "compliant". Applying this approach to the full cloud data set then accumulates statistics on the occurrence of "compliant" retrievals. In this way, the cloud field will be sampled correctly for each specific orbit type, including the co-variance of retrieval sensitivity to view / solar geometry and surface albedo

Some issues cannot be fully addressed using geostationary data (e.g. effect of pixel size smaller than that attainable by the SEVIRI (geostationary) data-set, geographical regions outside those seen by SEVIRI). These issues were addressed (in Task 4 only) by targeted analyses based on LEO cloud data from MODIS.

5.2 Cloud data used

The primary data selected for this analysis is that derived from MSG SEVIRI by the CM-SAF (archived at DWD). SEVIRI is a geostationary multispectral imager with a pixel size of 3 x 3km at the sub-satellite point, and observes a specific region of the world (illustrated in various figures below) every 15 minutes. This data was selected, as being the most suitable for the purposes of this project as it samples a wide range of geographical locations, at all times of day, and with a pixel size smaller than the threshold requirements for trace gas monitoring. One year of data was acquired by RAL, with assistance from colleagues at DWD. The cloud parameters obtained were cloud optical depth cloud height, cloud mask and cloud type. Although SEVIRI observes every 15 minutes, it was only possible to obtain data sampled every hour (at 45minutes past each hour) for the purposes of this project.

Results based on this dataset are complemented by an analysis of the corresponding year of MODIS data by SRON. MODIS extends the statistics to pixel sizes and geographical locations which are not possible to address with SEVIRI, and provides insight into the how sensitive the analysis might be to the choice of a specific instrument and cloud detection algorithm. MODIS level 2 Cloud Product (MOD06, collection 5), from MODIS Terra (10:30 descending node crossing time) were used.

5.3 General Approach

Geographical regions have been defined within which the cloud data set was sampled to generate statistics. We primarily consider 240 x 240 km regions centred on London, Madrid, Athens Kampala, Cairo and a location over the Atlantic (up-wind of Europe). The locations are shown in Figure 5-1. The table also indicates the area of a geostationary pixel over each region, relative to the area at 0°E, 45°N (the location at which the geostationary sounder spatial resolution / sampling requirements are defined in the MRD).

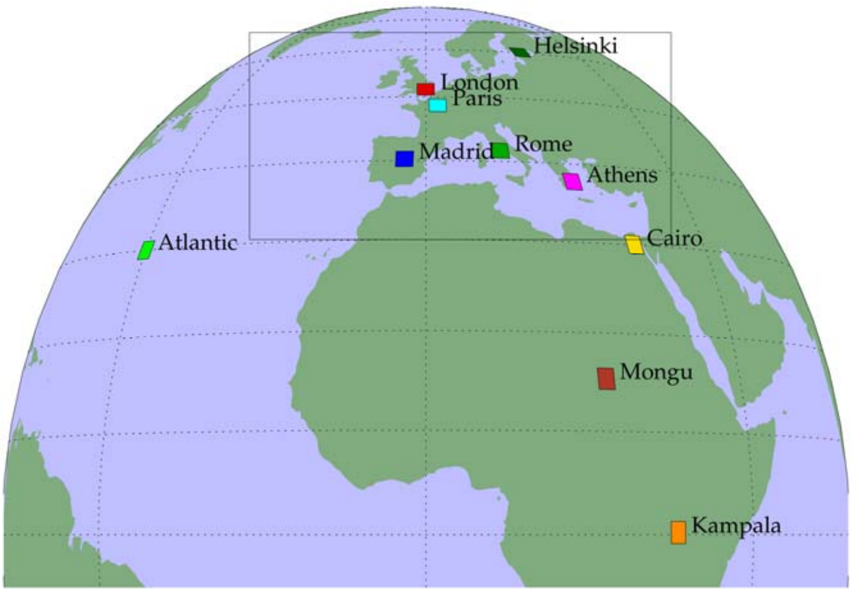


Figure 5-1: Regions for which cloud statistics have been generated based on SEVIRI data. Box shows the required coverage of the geostationary sounders

The statistics were generated based on hourly, full resolution CM-SAF data obtained on every day for 1 year, for the selected regions. Since the primary mission requirements relate to measurement of the troposphere, for air-quality applications, we focus here on determining a statistic, referred to as P1, the likelihood of obtaining at least one cloud-unaffected observation within a given field-of-regard (FOR), within a given time-window. P1 is determined as a function of

- Location
- Time of day and month of the of the year
- The time window over which observations may be acquired. Three periods are considered here:
  - 1 hour (the sampling interval of the CM-SAF data, so this is equivalent to instantaneous sampling)
  - 24 hours
  - Sampling during all sun-lit hour of the day (location and time of day dependent)
- The assumed pixel size
- The size of the FOR, i.e. the spatial area within which it is considered important to have at least one observation (e.g. the required spatial resolution of an L2 product).
- The acceptable level of cloud contamination in the scene. Cloud is parameterised as a function of fraction within the scene, mean optical thickness in the scene and mean cloud-top height. A scene may be considered ``cloud-unaffected'' if the fraction, optical thickness or height are below threshold values. Thresholds may be applied in combination.

In this study we focus on FOR sizes of 10, 20, 30, 60 and 120 km. 20km and 60km are of particular relevance as they match the threshold L2 requirements on most boundary layer and free tropospheric column products, respectively. We focus exclusively on a time window for P1 of 1 day.

For the purpose of tracking the evolution of a species throughout a day, another potentially relevant statistic is N1: The mean number of individual integration periods that have at least 1 cloud unaffected observation within the field-of-regard, over the whole time-window, provided at least 1 time-window has at least 1 cloud free observation. This complements P1 by providing an indication of how many time-slots are likely to be unaffected by cloud, once at least one time-slot has been identified as unaffected. Note that N1 will usually have a value from 1 to 24 (since it is based on hour statistics for a window of 24 hours). Only in the case of P1 being 0, would N1 be 0. One may also note that the mean number of hourly time-slots, which are cloud-unaffected within a day (over a given period and without the condition that at least one time-slot be free within the day), can be obtained by taking the product of P1 and N1.
Both statistics depend on how the field-of-regard (FOR) is assumed to be sampled by the instrument field-of-view (FOV) or pixel size. Here we assume the instrument regularly samples the field-of regard with contiguous coverage. I.e. the instrument cannot specifically target a cloud-free area.

Note that the geographical region for which statistics are computed is distinct from the FOR. Regions are always 240 x 240 km about a given location. Statistics are accumulated for all FOR within the region, effectively reducing noise on the estimated statistic. Figure 5-2 illustrates the meaning of FOR, pixel and region.

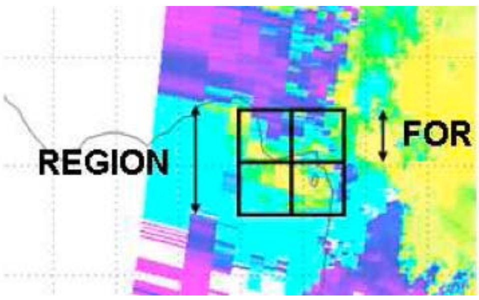


Figure 5-2: Figure shows a swath of polar orbit data. Each coloured tile represents a ground pixel or FOV (coloured tiles), which in this case increase in size toward the edge of the swath. The swath passes over a region which, in this case, comprises 4 fields of regard (FOR).

5.4 Using SEVIRI data to simulate different observing conditions

The SEVIRI cloud products can be used to simulate cloud fraction, mean optical thickness and altitude within the FOV of instruments with coarser temporal sampling and spatial resolution than SEVIRI itself. Here we use the dataset to simulate (for the regions identified above) these 3 cloud parameters observed in square ground pixels of dimension 10, 15, 20 and 50km, from the following platforms:

- Geostationary.
- Sun-synchronous polar orbiter (98° inclination, 820km altitude) with ascending node crossing times of 21:30 (as Metop), 10:30 (as MODIS), 13:30, 15:30 and 17:30.
- Non-sun-synchronous (NSS) polar orbit (55° inclination, 820km altitude). 4 such platforms are simulated, 90 degrees (or 6 hours) out of phase with each other. Because the swaths of successive orbits overlap in a range around 55 degrees N / S, each satellite would provide up to 5 observations of a given point on the ground, separated by the orbital period (approximately 100 mins). The local time during which this (approximately 8 hour) block of successive observations occurs varies through the year, so to obtain consistent coverage over the diurnal cycle at all times of year, multiple orbits would be required. A combination of 4 could approach geostationary sampling and would advance over GEO by covering all longitudes with dense temporal sampling (though only in a limited latitude band).

Polar orbiters are assumed to have a swath of ±66° (zenith angle at the ground) from nadir (2600 km swath width). The coverage of the polar orbit swaths is illustrated in figure 2.2.

In each case we distinguish two assumptions for how the FOV varies away from direct nadir viewing:

- *Fixed angular FOV*: The pixel size is defined at one view angle and varies away from it under the assumption the FOV has a fixed solid angle. In the geostationary case the nominal pixel size is here defined at 0°E, 45°N (in accordance with the MRD), so pixel sizes are smaller near to the sub-satellite point. For the polar orbiters, pixel size is defined at sub-satellite point and increases away from the orbit track.
- *Fixed FOV on ground*: The pixel size is assumed invariant of location, within the observed disk / swath.

It is considered that the former assumption is most reasonable for Sentinel 4/5 and therefore most statistics have been computed for this case.

Cloud fraction, mean optical thickness and mean altitude are explicitly computed for every pixel observed from polar orbit as follows:

- Each 1 hourly sampled SEVIRI file is read in turn.
- An orbit model is run to predict the location of observations by each orbit within ±30 minutes of the nominal time of each SEVIRI file.
- For each pixel which is within the disk defined by 70 degrees SEVIRI LOS zenith angle (at the ground), the SEVIRI (3km resolution) pixels are identified which fall within each pixel of the polar orbit, and the 3 pixel-specific cloud parameters computed.

This results in 1 polar orbiter file for each original SEVIRI file, containing the sub-set of the original data which would have been observed by such a sensor, at the appropriate resolution. Files have been created under both fixed-angle and fixed-on-ground FOV assumptions. SEVIRI has a sub-satellite pixel size of 3km, allowing simulation of pixels of dimension 10km over most of Western Europe.

Some limitations of the CM-SAF data that have consequences for the analysis and are noted below:

- The original CM-SAF data (at full SEVIRI resolution) flags fully and partially cloud pixels. As it is not possible to know the numeric fraction of “partially” cloudy scenes, both cases are considered as cloud fraction 1 in this analysis. Cloud fraction at coarser resolution is the mean of the individual values of 0 or 1 and so becomes a continuous value between 0 and 1, however, for the smaller pixels size simulated in particular, their will be a digitisation effect (e.g. the minimum non-zero cloud fraction for a pixel over northern Europe would be around 0.2).
- Cloud optical depth is only available when the sun is above about 20° elevation (as the product relies upon visible / near-infrared radiances).
- Cloud-top height is estimated day and night, however the retrieval sometimes fails (resulting in missing data) and this occurs more often during night.

Missing optical depths / heights are always assumed to correspond to optically thick / high cloud (i.e. the worst possible case) when used here to generate statistics.

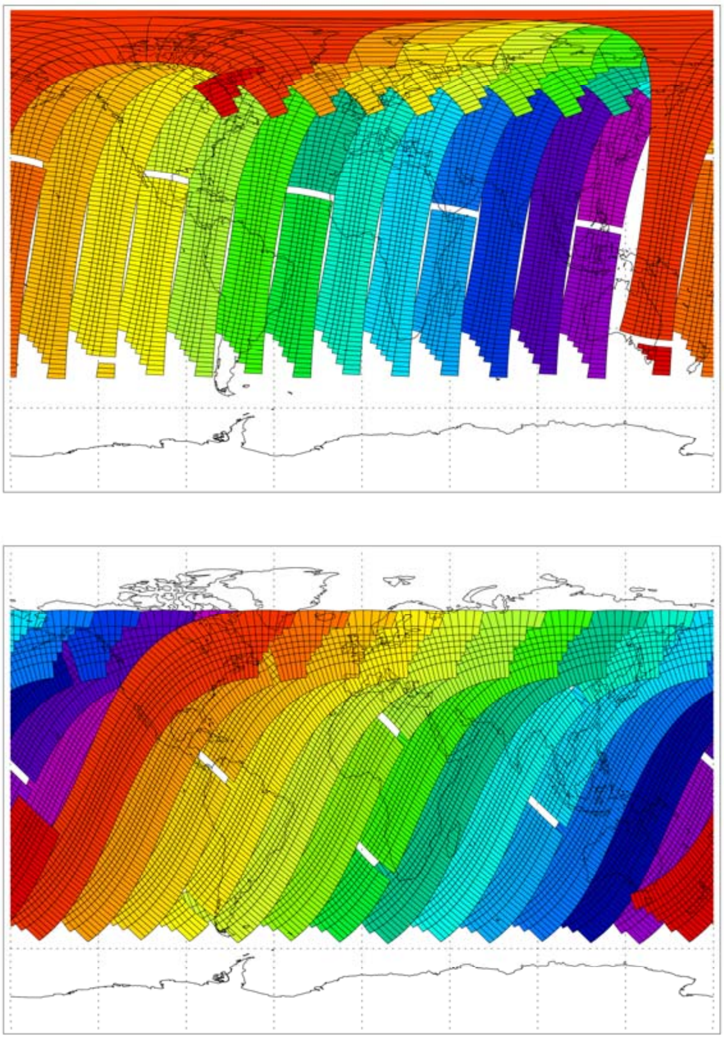


Figure 5-3: Simulated polar orbit swaths, where the solar zenith is less than 80 degrees on 1 July. The top panel shows a 9:30 sun-synchronous orbit. The bottom panel shows a 55circ inclination NSS orbit.

5.5 Calculation of statistics

Statistics P1 and N1 are computed on a monthly basis for the orbit, pixel and FOR options described above for the following cloud acceptance criteria:

- Scene must be completely cloud-free.
- Fraction <20% accepted (irrespective of height, optical depth).
- Fraction <5% accepted (irrespective of height, optical depth).
- Height <3 km accepted (irrespective of fraction, optical depth). (Such conditions are relevant as one might expect to observe the free troposphere despite the presence of low cloud).
- Cloud optical depth < 1 accepted (irrespective of height, fraction).
- Cloud optical depth < 5 accepted (irrespective of height, fraction).
- Cloud optical depth < 10 accepted (irrespective of height, fraction).

Statistics are computed for 24 periods and for only that part of the day for which the solar zenith angle is less than 80°, i.e. during daylight. The latter are relevant for L2 products relying on solar scattered radiation, though a fuller evaluation of the effect of view / solar geometry on L2 sampling is conducted in Task 5.

Statistics are only shown here for FOR which are at least as large as the nominal pixel size, since the utility of sampling a FOR with a pixel size larger than the FOR is not obvious. However note that, under the fixed angular FOV assumption, pixels can still be larger on the ground than the FOR. Such pixels will only be counted as entering into 1 FOR in determining the statistics, despite covering the area of more than one FOR. E.g. a cloud-free pixel which is nominally 10 x 10km which is stretched due to viewing across track to 10 x 20km will span 2 FOR. P1 (for the time window containing only these two observations) for this case will be 0.5 since only 1 FOR will be counted as having a cloud unaffected observation, despite the fact that the whole pixel (and therefore both FOR) is actually cloud free. Given the options, this is considered to be the most suitable approach for dealing with this issue (the alternative would not be appropriate as the FOR are not observed at the required sampling or resolution), however one should interpret with caution statistics for FOR comparable to the pixel size.

For reference, Figure 5-4, shows the variation of pixel size as a function of across track distance. Dotted lines indicate swath required to achieve approximately global coverage and the corresponding pixel size at the edge of such a swath. This effect explains why even the combination of multiple polar orbiters can sometimes have lower value of P1 (for 24 hours or whole day), than obtained with a single geostationary time-slot (see below).

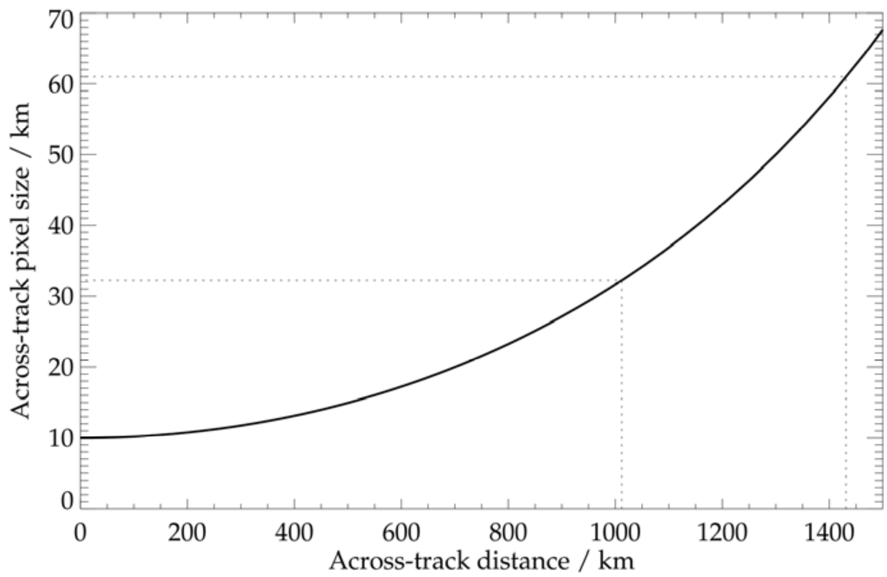


Figure 5-4: Variation of the across-track dimension of a ground-pixel observed from 820kmaltitude polar orbit, assumed a fixed angular FOV. Dotted lines indicate the required swath for complete global coverage (around 1500km across-track distance from nadir) and global coverage polewards of 45° latitude (N and S).

5.6 Example results for individual platforms

Figure 5-5 shows some example results based on geostationary orbit sampling for London.
Panels are as follows:

- Left: P1 for each hour of the day, i.e. the probability of obtaining at least 1 cloud unaffected FOR within the region, at a given time. Since SEVIRI is sampled every hour, this is the instantaneous cloud free probability. Different lines show different FOR / Pixel combinations (only those for nominal pixel size smaller than or equal to the FOR are shown).
- Centre: The P1 statistic for a time window of a day, shown as a function of FOR. In this case black lines show P1 considering all observations during the day and red lines show the case of daylight sampling only. Vertical lines in the left-hand plot indicate sunrise / sunset.
- Left: The N1 statistic.

The plots show clearly the expected strong dependence of P1 and N1 on the FOR and pixel size. Generally speaking, the cloud statistics show smooth behaviour as a function of time of day, usually without gross changes at the sunrise / sunset. Artefacts of the cloud-flagging algorithm use of visible channels might be expected to be apparent, but this is not generally the case.

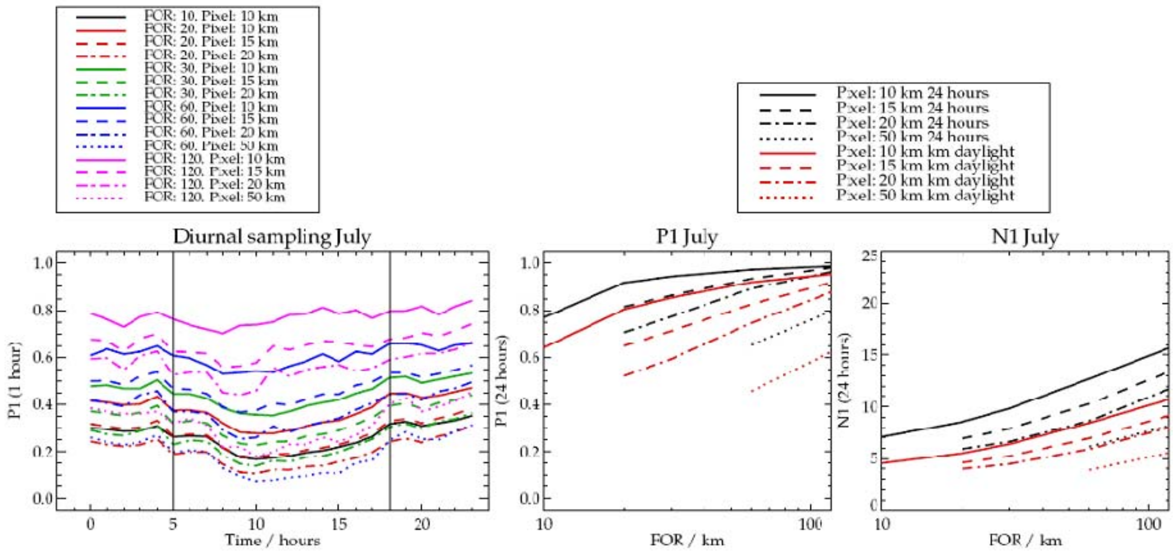


Figure 5-5: Example cloud-free sampling statistics for London, comparing various FOR and pixel size.

Differences in geostationary caused by different levels of allowed cloud contamination are shown in Figure 5-6 for a 10km pixel size over London. In each panel, the different lines compare the different cloud assumptions, as a function of FOR size. The following points may be noted:

- Clearly the extent to which P1 can be improved upon by relaxing cloud criteria depends on the starting value for completely cloud-free conditions: If the former is close to 1 then relaxing cloud criteria will make little difference. Hence the impact of accepting partial cloud is more powerful for polar orbit.
- Accepting cloud below 3km increases the probability of cloud-unaffected sampling considerably. However, this criterion makes little difference to statistics over Kampala which is dominate by higher level clouds.
- Even if P1 approaches 1 (or its maximum in the case of pixel size larger than FOR), N1 can still be increased by modifying cloud criteria, towards its maximum (the number of hours in the time-window).
- The daylight and 24 hours statistics (P1 and N1) for a single polar orbit are considerably worse than the case for GEO. This is due mainly to there only being at most two samples per day from polar orbit (from ascending and descending node), but also to the fact that complete global coverage is not obtained in a day, with the nominal pixel size because this is assumed to increase across-track (refer to Figure 5-4). Nevertheless, large values of completely cloud-free P1 are reached under favourable conditions, such as combining small pixel size with large FOR (e.g. 10km pixel, 120km FOR).

Figure 5-7 compares results for different regions. In each panel solid lines show 24 hour statistics and dashed lines show daylight. Not surprisingly, P1 and N1 associated with southern European and northern African locations are relatively large compared to those for London and the Atlantic.
London has the worst P1 values for all cases shown, followed by Kampala (quite closely), which is dominated by tropical convective cloud in most completely cloud-free cases.

Most attention focus in task 4 and 5 has been paid to the London, Kampala and Atlantic regions, as by being relatively cloudy, these are most sensitive to mission scenario.

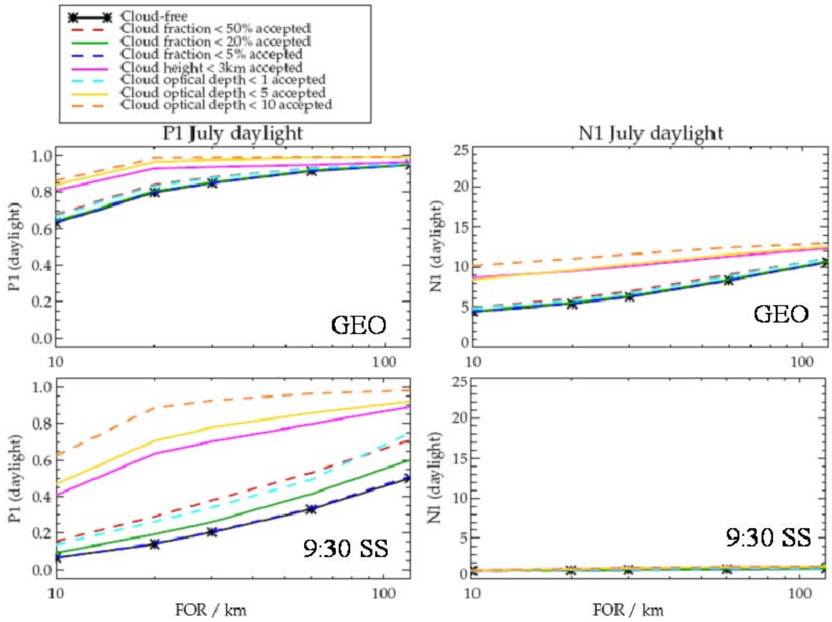


Figure 5-6: Comparison of P1 and N1 for daylight sampling with 10km pixel size over London in July, for various cloud acceptance threshold. Upper panels show results for geostationary orbit, lower panel show results for a single sun-synchronous (SS) orbit with 9:30 equator crossing time.

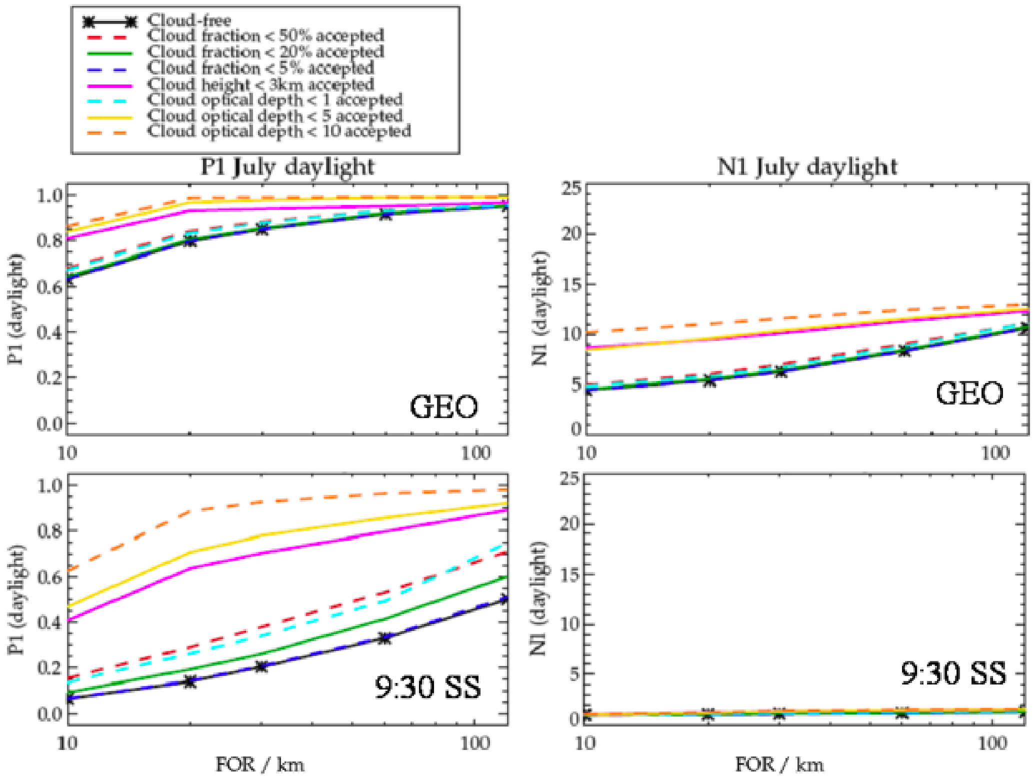


Figure 5-7: Comparison of P1 and N1, for a 10 km pixel, for 9:30 sun-synchronous polar orbit for various geographical regions, and considering 24 hours (solid) lines or daylight only (dashed) sampling. Upper panels show results for July and Lower panels results for December.

5.7 Example results for combined orbits

Here we compare directly the cloud-free sampling which can be obtained from a number of different orbit scenarios:

- Geostationary (GEO)
- Sun-synchronous (SS) orbits:
  - 9:30 descending node crossing time (as Metop)
  - Combination of both 9:30 and 13:30.
  - Combination of 9:30, 13:30 and 15:30.
  - Combination of 9:30, 13:30 and 17:30.
  - Combination of 9:30, 13:30, 15:30 and 17:30.
- The combination of 4 non sun-synchronous (NSS) polar orbiters, with inclination 55°, 6 hours out of phase.

Figure 5-8 illustrates how observations during a day and for multiple orbit combinations accumulate to provide the 24 hour and daylight values of P1 (London, July, 10km pixel). The instantaneous (hourly) geostationary P1 is shown as a black line, as a function of time of day (UT). Coloured lines underneath show the corresponding values for individual polar orbiters. Solid lines show sun-synchronous orbits, the local time of which can be identified by where P1 peaks during the day (e.g. red is 9:30). Note there is a spread of more than an hour about the nominal local time due to sampling at different points across track on different days within the 3 day period for approximate ground-track repeat.

Dashed lines show results from two of four the NSS orbits (12 hours out of phase). Arrows pointing to the left-hand axis show the values of P1, integrated over the 24 hour period for the orbit combinations indicated by the correspondingly coloured text. The GEO and 9:30 cases are intentionally shown the same colour as the corresponding lines in the main plot; different colours are used for the combinations (as lines in the main plot refer to individual orbits). Arrows pointing to the right-hand axis show P1 for daylight. The figure compares results for the "fixed angular FOV" assumption to those for "fixed FOV on ground". Note that in the former case (which is considered more realistic) the 9:30 polar orbit has a smaller daytime P1 than the individual hourly sample from the geostationary line at around 9:30. Assuming fixed FOV on the ground resolves this apparent inconsistency which is caused by the increasing pixel size away from nadir, where it is defined to be 10km.

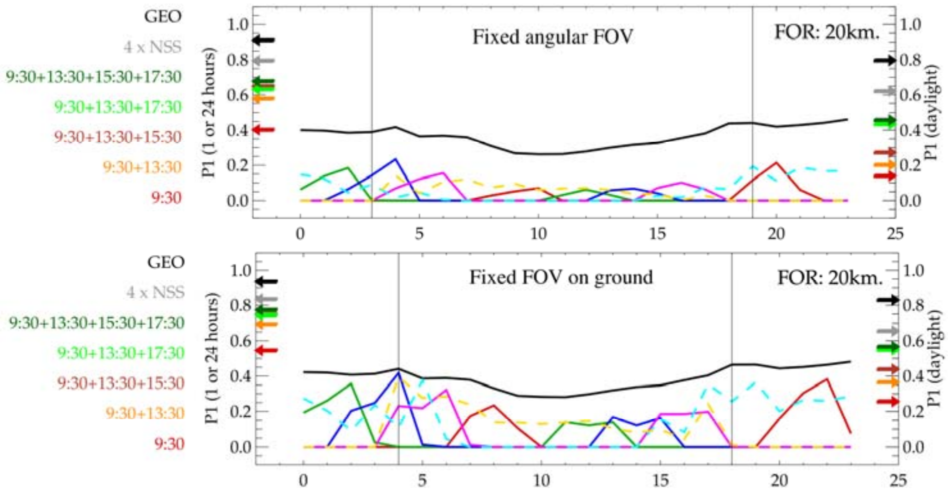


Figure 5-8 Illustration of the accumulation of P1 by combining polar orbits. Results shown are for a 10km pixel over London in July, considering a 20km FOR. Lines show the individual hourly sampling from GEO in black and from individual polar orbits in colour. Solid lines show SS orbits and dashed lines 2 example NSS orbits. Arrows pointing to the left hand axis show the accumulated P1 for various combinations of the orbit over the 24 hour periods. Arrows pointing to the left hand axis show P1 accumulated over sun-lit hours only (delimited by the vertical bars in the main panel).

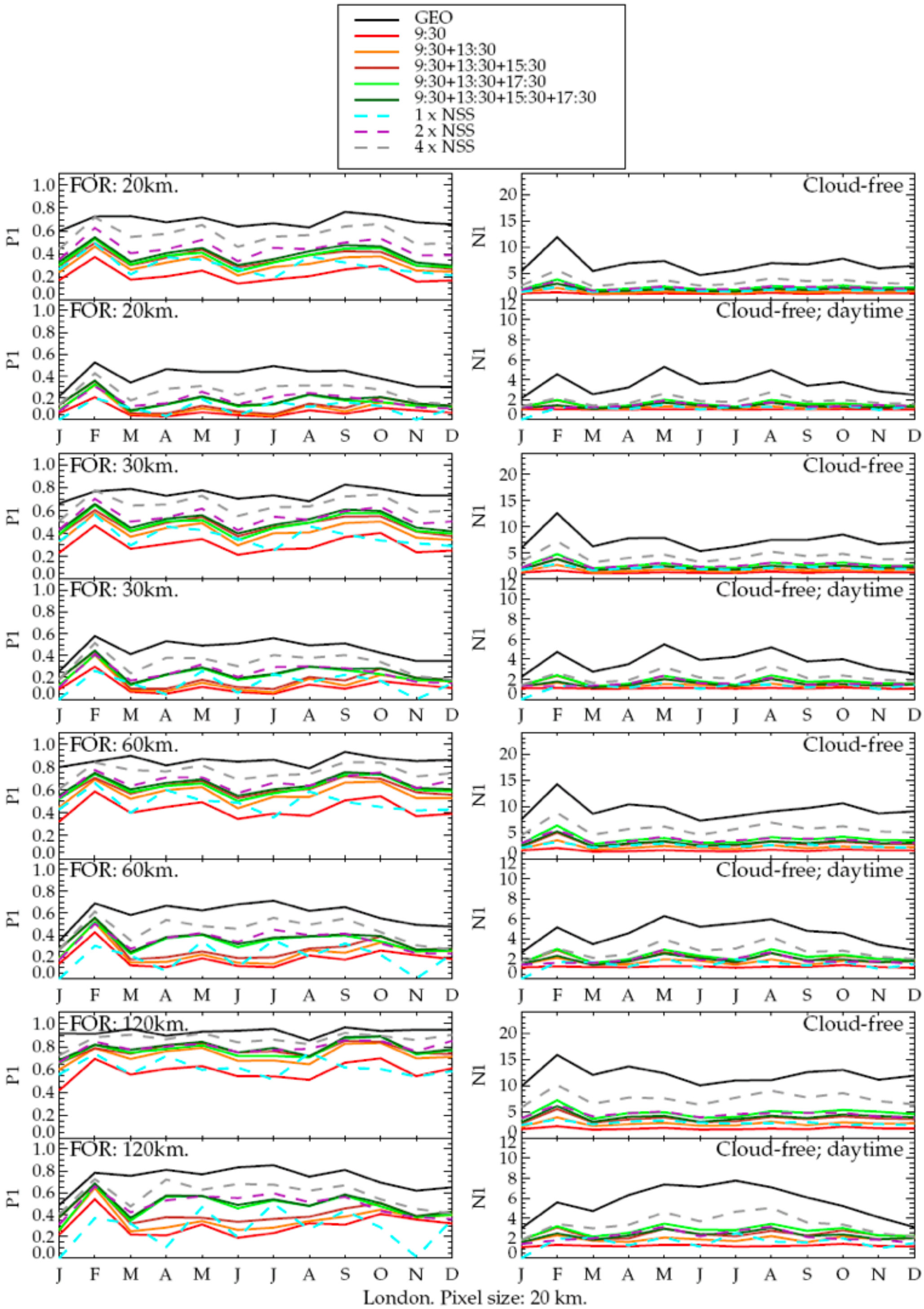


Figure 5-9: Monthly cloud-free sampling statistics for various orbits, for London, for a 20 km pixel size. Left-hand panels show the probability of obtaining 1 cloud free pixel over 24 hours (upper sub-panel) or during daylight (lower). Right-hand panels show the mean number of hourly samples found cloud-free, when at least 1 sample is cloud free in 24 hours or during daylight.

Figure 5-9 illustrates how P1(24 hours) and P1(daylight) vary during the year, together with the corresponding values of N1. Left hand panels show P1 and right-hand panels show N1. Each panel is split in two vertically, with the upper sub-panel showing results for 24 hours and the lower sub-panel showing results for day-light only. Panels from top to bottom show results for various FOR. The x-axis indicates the month by its initial letter, from January to December.

The following points may be noted from these plots for London:

- Geostationary almost always provides larger values the P1 and N1, even compared to 4 polar orbiters.
- Adding a fourth polar orbiter does not usually increase the P1 or N1 substantially, compared to considering only 9:30, 13:30 and 17:30.
- Apart from in winter, 17:30 seems to add more daytime cloud-free scenes compared to 15:30 (both considered in combination with 9:30 and 13:30). 15:30 improves only slightly on the 9:30 + 13:30 statistics.
- P1 for 4 NSS orbits approaches that of GEO. However N1 remains substantially smaller than GEO, though substantially larger than 4 sun-synchronous orbits.
- The progression through the year of the local times at which observations are acquired by a single NSS orbit is clearly reflected in the P1 statistic. 2 NSS orbiters (12 hours out of phase) no longer exhibit a pronounced variation, and the corresponding value of P1 is close to that obtained from 4 NSS orbits.
- N1(daytime) shows a strong seasonal variation, following the number of hours of daylight.
- February shows much larger P1 than January or March. This is related to favourable meteorological conditions during February 2008 over London (confirmed by the MODIS analysis), and therefore indicates the potential for inter-annual variability in cloud patterns to affect these statistics.
- In general, P1 varies from month to month but does not show a strong variation on longer time-scales (e.g. between summer and winter).

Analysing corresponding results for the Kampala and Atlantic regions showed that

- Kampala exhibits less seasonal variation than London or Atlantic.
- The gap between GEO and polar statistics is larger for Kampala than the other two regions, possibly because the GEO pixel size is actually smaller here than the nominal pixel size (defined at 45°N. However it should be noted that Kampala is outside the required region of Sentinel 4 observation.
- The NSS combination has little benefit over the sun-synch option for Kampala (as might be expected given the latitude of this location). Statistics for 50km pixel size are particularly poor for Kampala, presumably because of the large amount of small-scale cloud in the region.
- Statistics over the Atlantic have a pronounced seasonal variation, with P1 peaking in July.

5.8 Complementary analysis of MODIS data

A number of aspects affecting the sampling of cloud cannot be assessed by use of geostationary sensor data from SEVIRI including:

- sampling for pixel sizes smaller than SEVIRI;
- sampling of other regions of interest not observed by SEVIRI;
- the effect of the high line-of-sight zenith angle with which regions towards the edge of the disk (e.g. northern Europe) are observed by GEO compared to direct nadir observations from LEO.

These points have been addressed in this study by applying a similar analysis approach using MODIS cloud data instead of SEVIRI.

MODIS cloud statistics have been calculated for the following conditions:

- Regions around several cities in Europe (London and Madrid), Africa (Cairo and Kampala), US (San Francisco and Washington DC), China (Shanghai), and a region above the Northern Atlantic Ocean (-45°, 30°);
- Combinations of
    - FOR, *dfor*: 5, 10, 15, 20, 30, 60, 120 km
    - Pixel size, *dpix*: 1, 3, 5, 10, 15, 30 km
    - Allowed cloud fraction, *f*: 0, 0.05, 0.2
    - Allowed cloud optical depth, τ: 0, 1, 5

For this study we used the MODIS level 2 Cloud Product (MOD06, collection 5), which combines infrared and visible techniques to determine physical and radiative cloud properties. Cloud particle phase, effective radius, cloud optical thickness, and cloud integrated water path are derived at 1 km pixel resolution using the MODIS visible, near-infrared, and shortwave infrared bands.

The MODIS MOD06 product includes the MODIS level 2 Cloud Mask at 1 km pixel resolution. The MODIS cloud mask is based on a whole range of tests mostly thresholds applied on many channels ranging from visible to infrared and combinations of channels. If all tests indicate cloud free than the pixel is flagged ”confident clear”. If several or more tests fail then the mask has the value ”probably clear”, ”uncertain” and ”cloudy”, respectively. Most thresholds are a function of geolocation, viewing geometry and time of year.

This mask is clear-sky conservative, minimising clear detection, but missing clear regions that spectrally resemble cloud conditions. Known limitations of the MODIS cloud mask are (1) an aerosol-laden atmosphere maybe flagged as cloudy (indicated by a separate bit in the cloud mask); (2) thin cirrus (cot < 0.5) is not flagged in the cloud mask, but indicated by a separate bit; (3) incomplete or bad radiometric data creates holes in the cloud mask. The lower confidence values are most often found at the edges of clouds, and indicate partially cloudy scenes. In this study, we define “clear” when a simulated pixel (larger than 1 km) only contains confident clear MODIS observations (labelled τ99), and “likely clear” when no more than 20% of the MODIS observations are probably cloudy (labelled τ66).

The effect of high line-of-sight zenith angle has a noticeable effect on fraction of cloud-free observations. To illustrate this effect, we have collected one year of MODIS level 2 cloud mask data for a region above the Atlantic ocean: longitude between -40 and -50°, and latitude between 25 and 35°. We derived statistics for the fraction of cloud-free observations as a function of line-of-sight zenith angle using three selection criteria: only confident cloud-free observations, at-least probably clear, and non-confident cloudy.

Figure 5-10 shows that the fraction of cloud-free pixels decreases as a function of line-of-sight zenith angle. The number of confident cloud-free pixels is affected by the presence of Sun glint for positive line-of-sight zenith angles. Krijger et al. (2007) showed that the probability of finding a cloud-free observation decreases as a function of sensor resolution. They quantified this effect, based on MODIS data, representing one year of data averaged globally between 70°North and 70°South. They found that the fraction of cloud-free observations decreases from 33% at 1 km resolution (nadir) to 26% at 3.3 km resolution (LOS ±45°). Roughly equal to the results we have found when the probably cloud-free observations are included, indicating that the dominant effect is the increase in pixel size projected onto the ground, rather than a more subtle effect related to slant-viewing of 3D structured clouds.

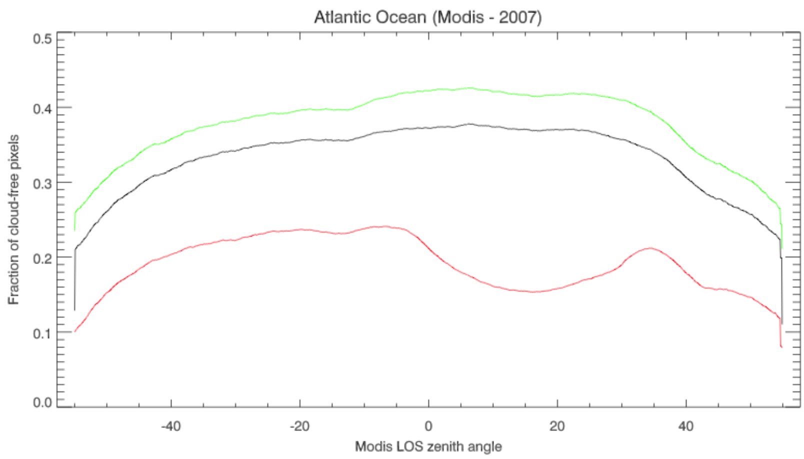


Figure 5-10: The fraction of cloud-free observations as a function of line-of-sight zenith angle, for a region above the Atlantic Ocean: longitude between -40 and -50°, and latitude between 25 and 35°. Three criteria are used to determine the number of cloud-free observations: confident clear, at-least probably clear, at-least probably cloudy, indicated by red, black and green, respectively

Examples of P1 for regions not observed by SEVIRI are shown in Figure 5-11.

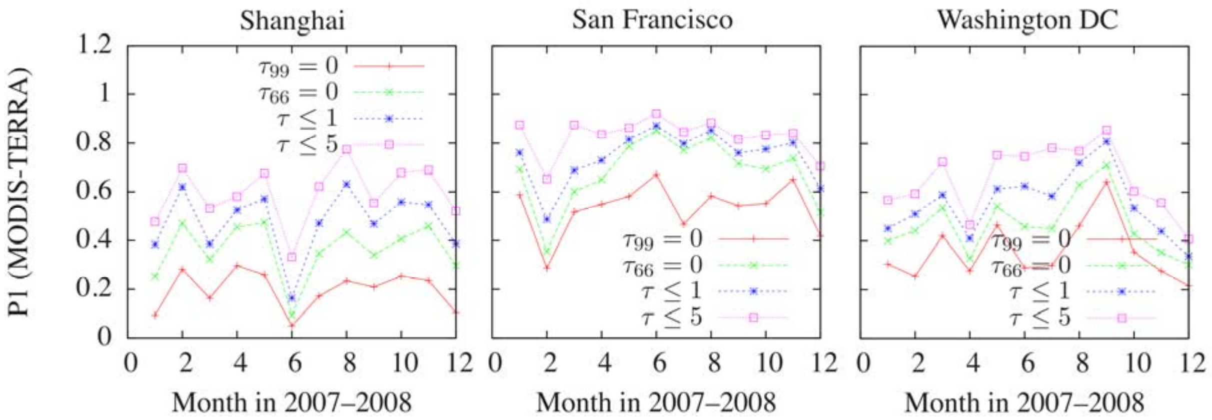


Figure 5-11: Example P1 statistics determined using MODIS data for regions not observed by SEVIRI. Each line shows a difference cloud flag / opacity criterion. Results are for an FOR of 30km and a pixel size of 10km.

5.9 Comparison of MODIS and SEVIRI

To establish the relationship between statistics derived from MODIS and SEVIRI, a subset of the MODIS statistics within the SEVIRI disk were compared against to equivalent statistics generated from SEVIRI, we compare P1(completely cloud free) generated from SEVIRI to MODIS statistics for the following cloud acceptance criteria:

- cloud free based on “confident clear” flag
- cloud free based on “probably clear” flag
- cloud optical depth < 1 and < 5 accepted
- cloud fractions 0, < 5 and < 20 accepted

Comparisons are made for varying FOR (10, 30, 60 and 120km) and a pixel size of 10km (which can be simulated by both instruments). The 10:30 ascending node crossing time orbit of MODIS has been explicitly simulated from the SEVIRI data for this purpose, and the same line-of-sight (swath) and solar zenith criteria are applied.

Example results are shown in Figure 5-12 which show P1 for varying FOR (indicated by the different colours). Each panel shows results for one of the above cloud-criteria applied to MODIS. (In each case the same completely cloud-free SEVIRI statistic is shown.) Solid lines show SEVIRI results and dashed lines show MODIS. Accepting COT < 5 results in generally much higher P1 than obtained from SEVIRI. This is as expected, as the SEVIRI cloud tests should certainly identify cloud down to low optical thickness.

The MODIS P1 based on the “confident clear” is always substantially lower than the SEVIRI based value. This occurs for all regions examined. This discrepancy will be due to a combination of “confident clear” flag falsely identifying clear scenes as cloud, and the SEVIRI flag missing some cloud (e.g. thin cirrus).

The agreement between SEVIRI and the MODIS “probably” clear case is in most cases remarkably good. The agreement is less good between May-September 2007 for London. In this case the COT <1 test agrees very well, indicating that the discrepancy might be related to the occurrence of thin cloud.

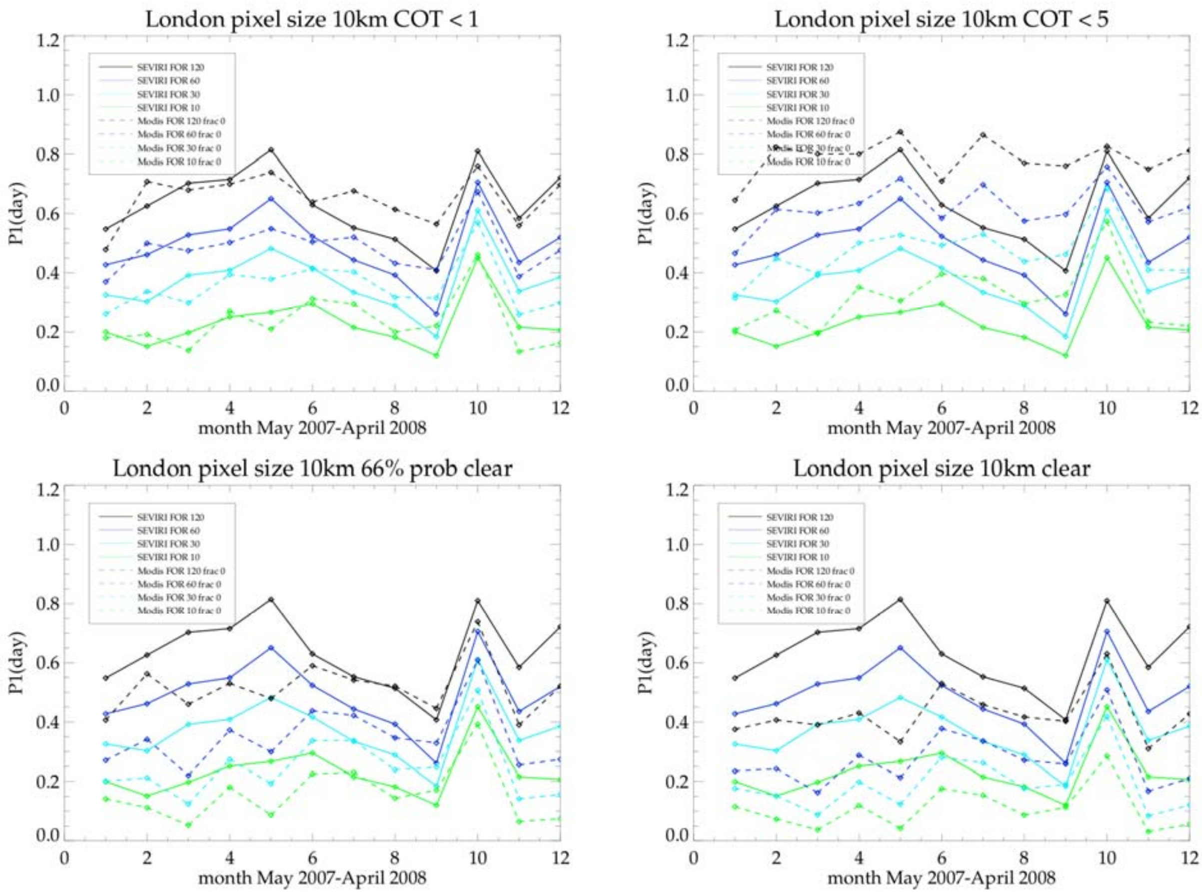


Figure 5-12: Cloud sampling probabilities for SEVIRI and MODIS for varying FOR for different cloud optical depth scenarios over and different cloud clear probabilities London

5.10 Summary and conclusions from task 4

Using SEVIRI data sampled hourly for one year, the statistical occurrence of cloud-unaffected observations has been assessed as a function of geographical region, season and time of day, pixel size and field-of-regard, observing platform, and various levels of allowed cloud contamination of a scene (optical depth, fraction and height thresholds).

The SEVIRI dataset (generated by the CM-SAF) was selected as this allowed the widest range of orbit conditions to be simulated possible with any single data set. This analysis was complemented by an analysis of MODIS data to primarily investigate regions not viewed by SEVIRI. MODIS data was also to confirm that SEVIRI data was appropriate for simulating polar observations of key European cities such as London.

Throughout the analysis it was recognised that the use of a simple cloud flag from any single instrument (or algorithm) could bias statistics. Cloud occurs at widely varying spatial scales, with widely varying optical thickness, and any flag indicating “clear” or “cloudy” will divide these classes in different ways depending on the sensitivity of the instrument and the intended purpose of the flag. E.g. a flag intended to identify scenes that are unambiguously clear may often falsely identify clear scenes as cloudy. This consideration motivated the assessment of various levels of cloud contamination (fraction, optical depth thresholds), which are expected to be less sensitive to choices implicit in a binary cloud flag. Also with this in mind, MODIS and SEVIRI statistics were compared (for conditions which could be simulated from both datasets) to establish the relative behaviour of “cloud-free’ statistics based on their respective cloud-flags. This comparison has quite clearly established that the SEVIRI cloud-flag is not strongly conservative, and matches most closely the MODIS "probably clear" classification. The quality of this agreement with MODIS demonstrates that the statistics are soundly based.

There are nevertheless some limitations of the SEVIRI data which will affect results to some extent:

- Optical depth information is only available when the solar elevation is sufficiently high. It is therefore not available at night, or during December for relatively high latitude locations (e.g. London).
- At some locations / time of year, the cloud detection algorithm reports relatively low amounts of cloud around sunrise / sunset, which are presumably spurious. This will introduce a bias in favour of observations which sample around this time.
- Comparisons to MODIS indicate that SEVIRI under-detects optically thin and / or low-fraction cloud. "Cloud-free" statistics based on SEVIRI may therefore be optimistic if one is interested in observations which are very sensitive to clouds.

If feasible, it would be desirable to improve upon these deficiencies in a future re-analysis.

The general dependencies of cloud-unaffected sampling were as expected:

- Smaller pixel sizes lead to a much higher probability of obtaining a cloud-unaffected scene.
- This probability also increases if one requires the cloud-free scene within a larger field-of regard.
- Combining observations from multiple times of day increases the probability of obtaining one observation and the number of individual unaffected observations.
- Allowing partial, thin or low cloud in a scene increases the probability of an unaffected observation.
- Results depend strongly on location and (generally to a lesser extent) on time of year.
- There is some dependence on time of day, though this depends on location. For sun-synchronous orbits, statistics indicate an early morning orbit (such as Metop) would suit locations like Kampala, while an orbit around mid-day would provide better cloud free sampling of the Atlantic region.

A single polar orbiter, with wide swath and small (10 km) pixel size can provide high cloud free sampling probability if the pixel size is small and one is only interested in obtaining an observation within a large FOR. (E.g. even for relatively cloudy London, cloud-free P1 of 0.8 is reached for 10 km pixel size and 120 km FOR assuming day and nighttime observations are useful). The benefit of multiple observations during the day becomes dramatic if the observation technique requires daytime observations and in particular for smaller FOR / larger pixel size.

The relative performance of geostationary and polar observations was found to depend critically on how the field-of-view (pixel size) is assumed to vary away from the nadir direction. Simulations were performed for a nominal pixel size defined at nadir for a polar orbiter and at 0°E, 45°N for a geostationary sensor. Away from these locations it was assumed that angular field-of-view remained fixed. This leads to an increase in pixel size across-track for the polar orbiter and towards the edge of the disk for a geostationary (GEO) sensor. However for the locations considered here, the latter is much less dramatic than the variation across-track of a polar orbiter, when considering the swath necessary to obtain global coverage of all longitudes in a single day. Because of this consideration, the probabilities obtained from polar orbit are worse than one might naively expect considering an instrument with a particular pixel size and a swath large enough to cover all points on the globe. It should be noted that these cloud statistics are affected in two ways by the increasing pixel size across-track:

- As the area increases, the probability of it containing some cloud increases. To some extent this effect will be reduced if one accepts some level of fractional cloud cover in a scene.
- If the pixel is becomes larger than the FOR, then the observations under-sample the spatial scale at which observations are required. Here, a pixel is only considered to contribute information on one FOR so, even if a region is always completely cloud free, the reported probability of obtaining a cloud free FOR will be less than 1, because not all FOR have an associated cloud-free pixel.

It is considered appropriate for Task 4 and 5 that both these effects be included in the statistics, as alternatives would be somewhat unrealistic. Achieving pixel size fixed on the ground may be impractical to achieve with the technology considered for Sentinel 4/5 sensors, and even if it were possible this would likely imply a reduction in signal to noise which would potentially also affect the sampling of useful data (and be very difficult to simulate here). Allowing pixels larger than the FOR to count towards all FOR within the area spanned by the pixel would be misleading as the FOR is intended to represent the resolution at which observations are needed.

If GEO and polar have the same nominal pixel, then is almost all circumstances the GEO provides larger values of P1 and considerably larger values of N1. This is true comparing GEO to up to a combination of four sun-synchronous orbiters. Over the latitude range for which the non-sun synchronous (NSS) orbit is optimised (around 55° N), four such sensors provide P1 comparable to GEO, and in some cases marginally higher. Although not explicitly simulated here, it is probable that only 3 NSS sensors separated by 8 hours would be sufficient to achieve close to this performance (since the period over which one NSS sensor provides frequent sampling of the same point on the ground is approximately 8 hours).

Adding 13:30 sun-synchronous polar orbit to the 9:30 leads to a large increase in cloud-free sampling probability. Adding the 17:30 orbit adds further useful observations (provided these are sun-lit when relevant). Little seems to be gained is gained by adding the 15:30 orbit to 9:30 + 13:30.

It must of course be recognised that GEO cannot provide global coverage and, in order to obtain the smaller pixel sizes (and hourly sampling) considered here, only the European region can be covered. Hence if global observations are required, then GEO should always be considered as adding to observations from polar orbit.
The capability of 3-4 NSS sensors to provide sampling comparable to GEO at all longitudes should be viewed in this context. Furthermore 3-4 sun-synchronous orbits will provide high sampling of high-latitudes (around 82°N) comparable the NSS orbits around 55°N a region which is impossible to sample from geostationary orbit.

Further discussion on the balance between orbit options is provided in Task 5, on the firmer basis of level 2 product sampling statistics.

6 Optimisation of Mission Scenarios

6.1 Introduction

As described in the overview to Task 4, above, task 5 extends the analysis developed in Task 4 to explicitly compute P1 and N1 for the sampling of level 2 retrieved products which are able to satisfy user requirements. This mapping between cloud occurrence and other geophysical criteria is accomplished by using the simulated orbits generated in task 4, applying on a pixel-by-pixel basis an operator which determines whether a particular scene is compliant with user requirements.

6.2 L2 retrieval sensitivity Look-Up-Tables

Each task 3 retrieval team was tasked with populating a multi-dimensional look-up-table (LUT) which defines the region in which a retrieval meets user requirements, as a function of the cloud parameters which affect retrieval sensitivity (i.e. fraction, opacity and height), together with relevant view / solar geometry and surface characteristics. This LUT is then "flown" through the cloud-dataset and for each individual observation (integration period/ field of view) the correct parameters for the orbit are determined and the LUT used to determine whether or not the retrieval is "compliant". Statistics on the occurrence of "compliant" retrievals are then accumulated by applying this approach to the full year of data used in Task 4. In this way, the cloud field will be sampled correctly for each specific orbit type, including the co-variance of retrieval sensitivity to view / solar geometry and surface albedo.

Precise details of the LUT depended on the L2 product and associated retrieval technique. The following LUTs were provided:

- Troposperic H_2O from TIR (IFAC)
- Tropospheric O_3 from UVN (RAL and KNMI)
- Tropospheric O_3 from TIR (RAL)
- Nitric acid and PAN from TIR (Univ. Leicester)
- CO from TIR (Noveltis / LPMAA)
- CO from SWIR (SRON)
- Aerosol optical thickness from 3MI (SRON)
- NO_2, CH_2O and SO_2 from UVN (BIRA)

Because of the complexity of performing simulations to comprehensively assess the sensitivity of a retrieval to cloud, it has not been possible within the duration of Camelot to explicitly generate statistics on all L2 products expected from S4/5. It should also be borne in mind that (while being, by far, the most suitable data-set available for present purposes) the SEVIRI cloud product may underestimate optically thin cloud that might still pose problems for most challenging products such as height-resolved aerosol from the A-band, CH4 and CO2. For such species the cloud-free sampling statistics provide a probably optimistic estimate of the likely cloud-free sampling.

In the case of the O_2 A-band sounder retrievals of height-resolved aerosol, it was noted that performance is strongly dependent on observing conditions and is improved at relatively low solar elevation, because of the favourable scattering geometry for the aerosol signal. It is therefore of potential interest to analyse statistics of sampling cloud-free when the solar elevation is low. We therefore generate P1 and for cloud-free conditions and solar zenith angle in the range 60 - 80°, in addition to the standard cloud-free statistics and the explicitly modelled L2 sampling.

Cloud sensitivity LUTs for several species, namely PAN, CH2O and SO2, were generated simulated but were not used in generating compliant-sampling statistics as their basic, cloud-free errors were already non-compliant with user requirements. This should not be taken to imply such retrievals may not be useful, only that this mismatch between requirements and cloud-free errors could not be accommodated in the task 5 analysis.

Details of the LUTs are provided in the Task 5 report. Figure 6-1 illustrates an example LUT for UVN tropospheric column ozone (simulated by RAL). In these simulations full multiple scattering code has been used, together with optical models to prescribe the singles scattering properties. The low cloud is assumed to be water with effective radius 10 microns and Mie calculations, assuming a standard size distribution, are employed to predict the optical properties. Errors due to imperfect knowledge of cloud properties were estimated in addition to assumed instrumental errors (consistent with the MRD). Results here show typical patterns exhibited by most of the L2 sensitivity LUTs:

- Errors vary with view / solar geometry such that retrievals are not possible under some observing conditions irrespective of cloud.
- Depending on observing conditions cloud may be tolerated if it is thin and / or occupies a small fraction of the scene, otherwise requirements cannot be met.
- Typically high level is associated with a reduced range of opacity / fraction consistent with a compliant retrieval.

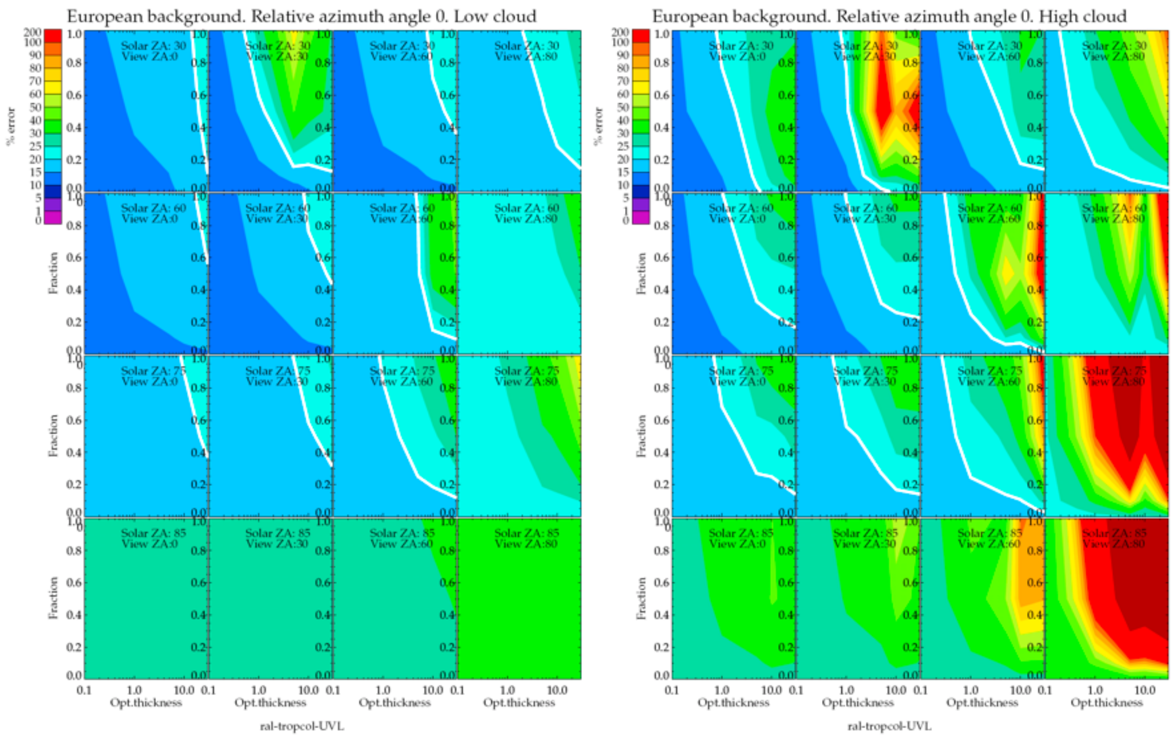


Figure 6-1. Task 5 retrieval sensitivity LUT for tropospheric column ozone from the UVN. Panels show the % uncertainty on the retrieved ozone column as a function of cloud optical thickness (x-axis) and cloud fraction (y-axis), for a specific viewing geometry defined by solar zenith angle (varying top to bottom) and view zenith angle (left to right). All results here are for a relative azimuth angle of 0^o. On the left, results for a low (<3km) cloud are shown and on the right, results for a high cloud are provided (>3km). The white line contour in each panel indicates the user requirement, below which the retrieval is considered compliant.

6.3 Example results

Bearing in mind user requirements and following results of task 4, the potential data-space to be optimised is restricted as follows:

- Locations London, Atlantic and Kampala are focussed on as they each have distinct patterns of cloudiness throughout the day and year. Furthermore they have relatively high levels of cloud compared to some of the other scenarios considered in T4 and therefore are more likely than e.g. Madrid, Athens, Rome to drive the optimisation of the mission to minimise cloud contamination. It must be borne in mind however that Kampala is characteristic of regions outside the expected observation area of the geostationary sounders of interest here. (While the Atlantic region in actually also outside this region, it is still directly relevant for both GEO and polar platforms as it will represent characteristic meteorology that will be observed from both platforms.)

- Pixel size 10 and 15 km are required (and likely to be in the range achieved) by the S4/5 sounders of interest here (GEO and polar). Larger pixel sizes remain of some interest for reference to existing sensors.
- FOR 20 and 60 km are of particular interest since these correspond to the threshold horizontal resolution user requirement for boundary and tropospheric column products, respectively. Even if specific boundary layer products are not considered explicitly here (LUTs relate to the more feasible tropospheric column), the 20 km FOR requirement is presumably relevant to species where the tropospheric column is particularly required to be sensitive to the boundary layer (e.g. NO_2, SWIR CO, aerosol).
- Combinations of GEO with polar observations yield results for P1 and N1 which are almost identical to GEO alone (where GEO provides observations). We therefore do not explicitly show results for different combinations of GEO and polar platforms. The only case shown here is GEO + 9:30 + 13:30, which is explicitly simulated as being the "baseline" case of MTG + Post-EPS + NPOESS, however results are to all intents and purposes identical to GEO alone or any other combination with polar orbits.
- Results for FOR smaller than the nominal pixel size are not shown.
- Results shown here are based on the assumption that the pixel size increases away from nadir assuming the angular field-of-view to be fixed. The issues raised under Task 4 regarding this assumption should be borne in mind (see Task 4 conclusions). Example results for assuming the pixel size is fixed on the ground are included for London only in the Task 5 report.
- In most cases, seasonal dependencies on cloud-free sampling are quite weak, so conclusions can largely be drawn from annually averaged values of P1 and N1 (i.e. the mean of the monthly P1 and N1 values over the year).

Plots comparing the monthly P1 and N1 statistics for different orbit combinations, for a specific region, FOR, pixel size and level 2 product are provided in the Task 5 report. Examples are shown here in Figure 6-2 and Figure 6-3 for tropospheric column NO_2 (UVN) and boundary layer column H_2O (TIR), respectively.

Orbits shown are:

- 9:30 sun-synchronous.
- 9:30 + 13:30 sun-synchronous.
- 9:30 + 13:30 + 17:30 sun-synchronous. As noted above, this is effectively equivalent to the combination also including 15:30.
- 4 Non-sun-synchronous (NSS) orbits, separated in phase by 6 hours. This is expected to provide similar results to 3 NSS orbits separated by 8 hours.
- 9:30 + 13:30 sun-synchronous + GEO. As noted above, for a specific location, this is effectively equivalent to GEO alone or in combination with any of the polar orbit options. (Of course the polar orbits considerably extend the geographic coverage of the GEO.)

Annual average values of P1 and N1 are summarised in Figure 6-4, Figure 6-5 and Figure 6-6 for the London, Kampala and Atlantic regions. The three pixel size / FOR combinations are shown from top to bottom in order of decreasing value of P1, i.e. P1 for any given orbit / L2 product is highest for pixel/FOR size 10/60km, and smallest for pixel/FOR size 20/20km. Other combinations are provided in the Task 5 report. Note 3MI aerosol simulations are only shown for the 10km pixel size (even this is larger than the instrument would provide).

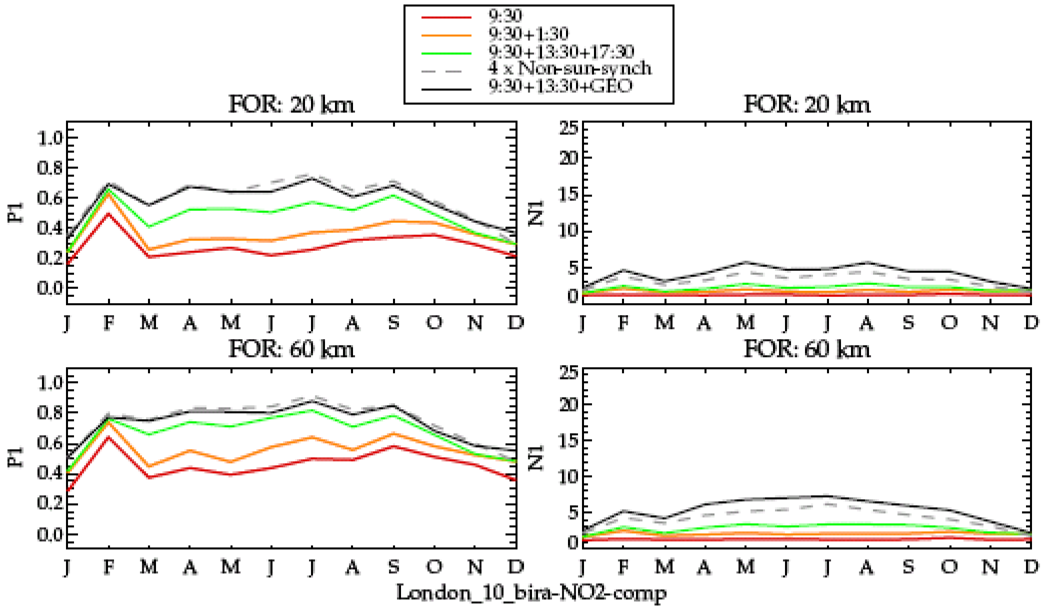


Figure 6-2. NO_2 sampling statistics for various orbit combinations, for 10 km pixel over London.

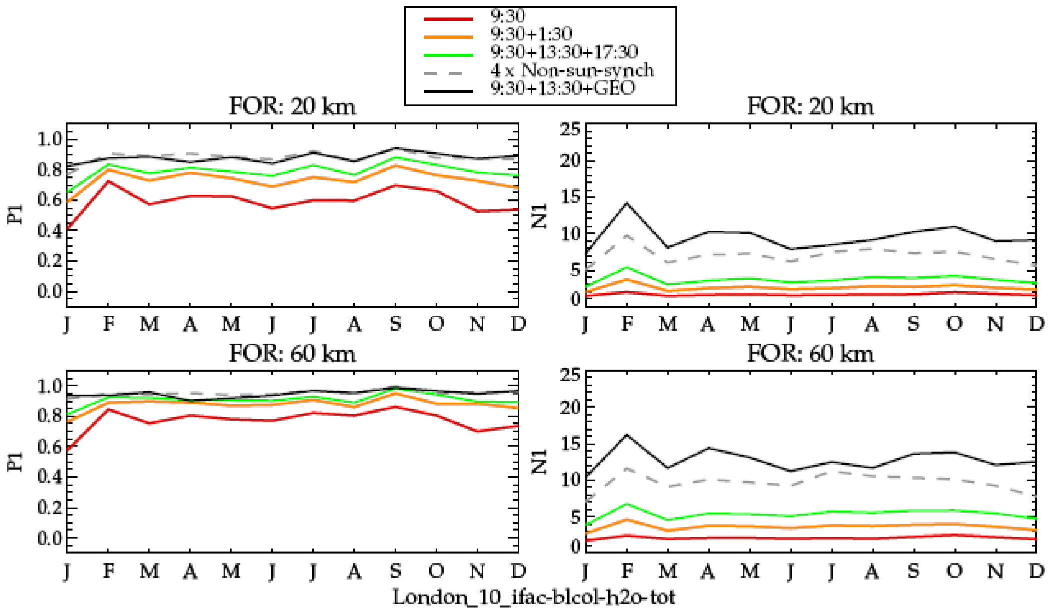


Figure 6-3. Boundary layer water vapour sampling statistics for 10km pixel over London.

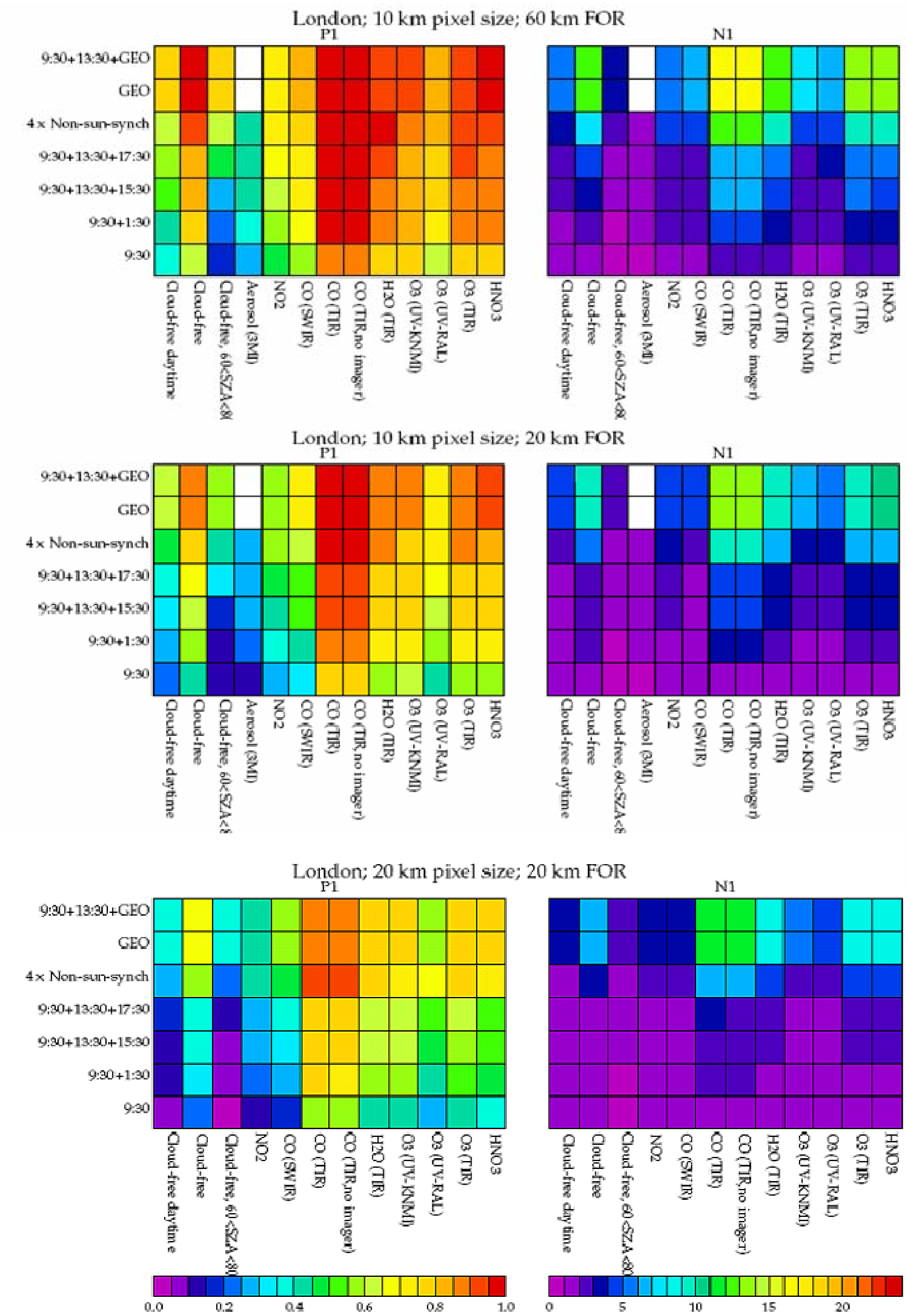


Figure 6-4. L2 Sampling summary for 3 combinations of pixel size and FOR; London.

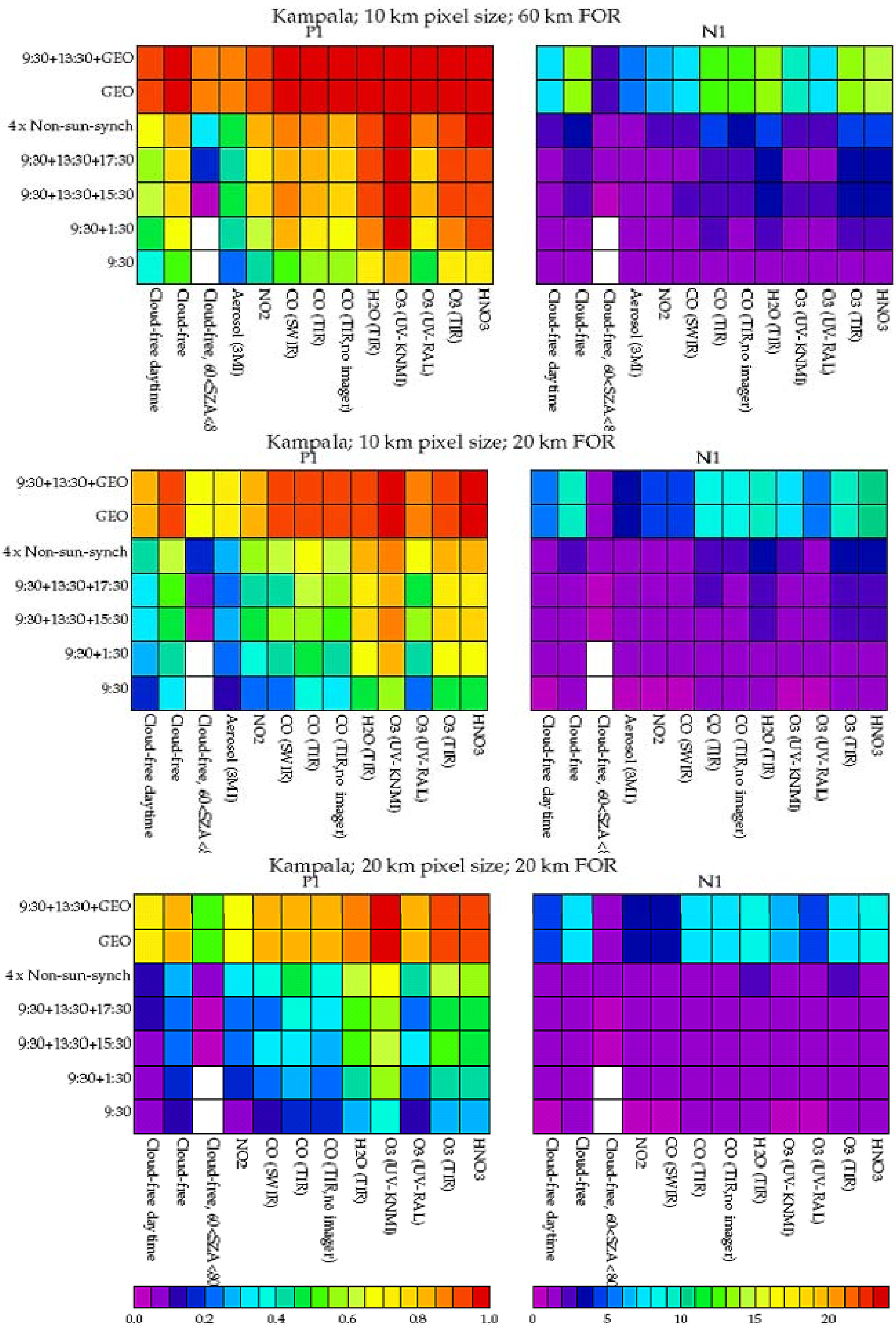


Figure 6-5. L2 Sampling summary for 3 combinations of pixel size and FOR; Kampala.

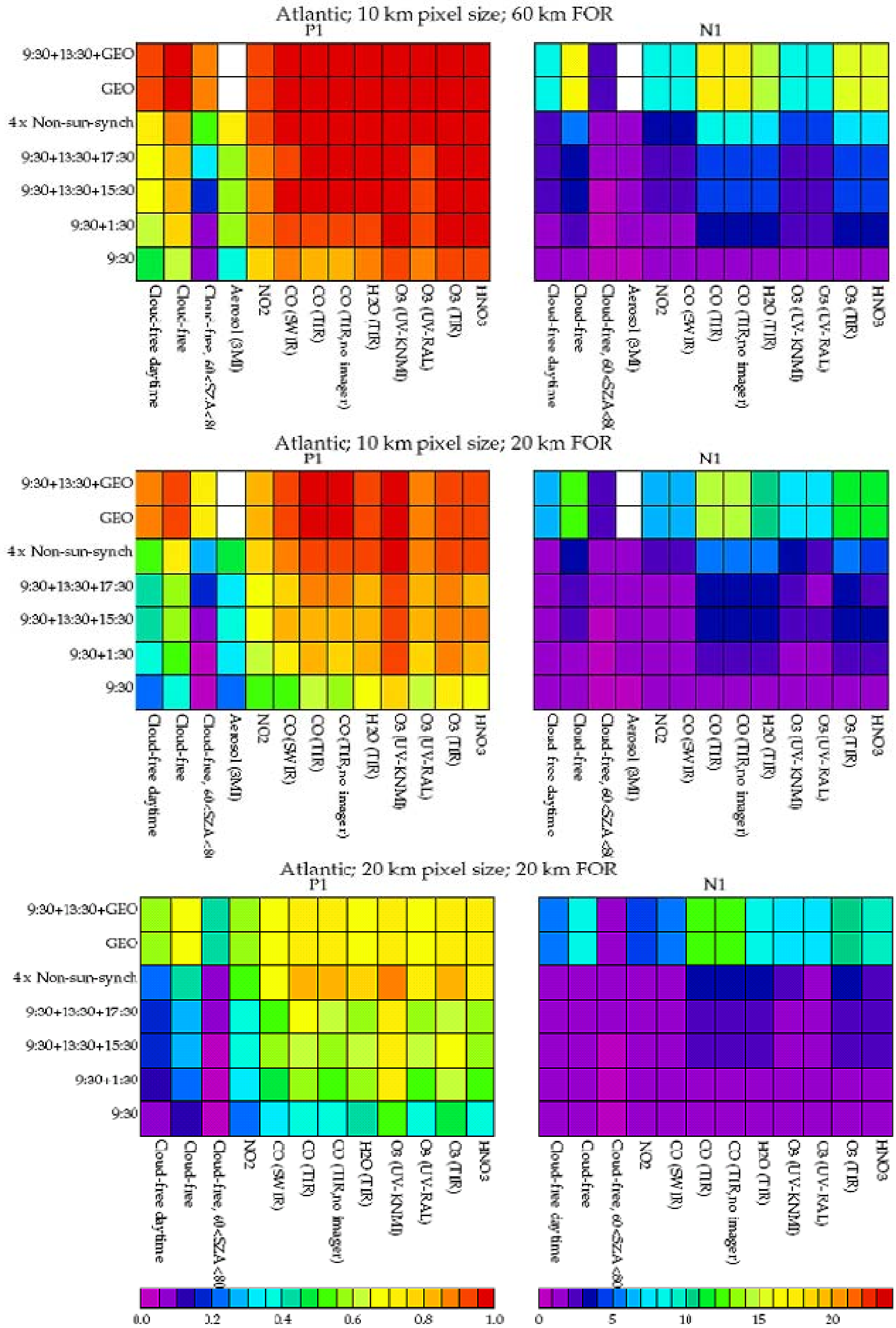


Figure 6-6 L2 Sampling summary for 3 combinations of pixel size and FOR; Atlantic region.

6.4 Discussion and conclusions

The general behaviour of the L2 product sampling statistics follows that of the cloud-unaffected sampling statistics reported in T4:

- The basic dependencies of the sampling statistics are as might be expected:
  - Smaller pixel sizes lead to a higher probability of obtaining a compliant scene.
  - This probability also increases if one requires the compliant scene within a larger field-of-regard (FOR).
  - Combining observations from multiple times of day increases the probability of obtaining one observation and the number of individual unaffected observations.
- Results depend on location and, to a lesser extent, on time of year.
- The assumption that the field-of-view (FOV) is a fixed solid angle, so that pixel size increases away from nadir, has a strong impact on the polar orbiter statistics in particular. However this assumption is considered most relevant of the possible alternatives.
- Under most circumstances (especially under the fixed-angular-FOV assumption), the geostationary platform provides the highest values of P1, though this may be marginal compared to 3 sun-synchronous or non-sun-synchronous (NSS) orbits.
- Geostationary orbit generally provides substantially higher values of N1 (in the region observed by the GEO platform).

As discussed, results here focus on pixel sizes in the range 10-15 km (matching the MRD) and FOR of 20 and 60 km, which correspond to the threshold user requirements on boundary layer and tropospheric column horizontal resolution, respectively.

Cloud-free sampling statistics were complemented by level 2 (L2) sampling statistics, which were generated using look-up-tables to summarise the sensitivity of each product to cloud as well as other factors such as viewing geometry and surface properties. Look-up-tables were used to identify on a pixel-by-pixel bases whether retrievals for a given scene / product would be compliant or not with user requirements.

Applying L2 sensitivity look-up-tables to simulated scenes, changes the relative importance of these effects by (a) allowing partial / thin / low cloud to be accommodated, thereby increasing the instantaneous probability of a cloud-unaffected observations and reducing the benefit (for P1) of sampling more frequently (b) introducing view or surface dependency which affects both cloudy and cloud-free scenes. Relative to their cloud-free values reported in Task 4, effect (a) will tend to increase P1 and N1 while effect (b) will tend to reduce them. However, effect (a) dominates for most species and locations, so tending to reduce the apparent benefit of adding geostationary observations or combining multiple polar orbits.

An important point to note is that by having a pixel size in the range 10 - 15 km, the Sentinel 4-5 sounders will greatly advance over existing UV/SWIR sounders. With a pixel size of 10 km, considering a FOR of 60km (the threshold for tropospheric column retrievals), a single 9:30 sun-synchronous orbit such as Metop / Post-EPS will provide annual average P1 which is generally above 0.7 for most thermal-infrared species, and above 0.5 for UVN/SWIR species (other than aerosol).

Combining two polar orbits at 9:30 and 13:30 substantially increases these figures, so the margin for improving P1 for by adding further observations is relatively small compared to requiring completely cloud-free scenes. If multiple observations are required within the day, however, geostationary observations provide the highest values of N1, closely followed by the NSS combination (for mid-latitude for which the 55° inclination is optimised).

L2 sampling statistics for the TIR species simulated here are quite similar to each other. H_2O, O_3 and HNO_3 in particular have very similar values of P1 and N1 for the same orbit combination and location. This is perhaps not surprising given the similarities in the behaviour of the LUTs illustrated in chapter 2, however it does indicate a robustness in the results given that these have been obtained by different groups using different retrieval codes. CO (TIR) sampling statistics are usually somewhat larger, reflecting the ability to deal successfully with low, optically thick cloud in the assumptions underlying that LUT. There is little apparent benefit in these results from adding the use of the imager to the CO-TIR observations.

For these TIR species the following further points are noted:

- Seasonal variations in P1 and N1 are weak for all TIR species (the strongest variations appear over the Atlantic).
- Combining 9:30 and 13:30 sun-synchronous observations substantially increases P1 for the relatively cloudy regions Kampala, Atlantic and London.
- Regions Madrid and Cairo have P1 above 0.8 for the 9:30 orbit alone (except for the more challenging case of FOR 20 km, pixel size 15-20 km).
- For most pixel sizes and FOR (i.e. unless pixel size is relaxed to 20 km and the FOR is also 20km), there is little increase in P1 obtained by adding a third polar or GEO orbit to the 9:30 + 1:30 case. (GEO would add significantly to sampling over Kampala, however this region is not within the observation area of the S4 geostationary sounders.)
- Four NSS orbits separated by 6 hours (and presumably 3 NSS orbits separated by 8 hours) give sampling similar or (in the case of Atlantic in particular) better than GEO.
- The benefit of GEO (or combining more than 2 polar orbits) lies therefore primarily in increasing N1. However, whether this may not be an important advance for the TIR column amounts, which are relatively insensitive in the boundary layer (where user requirements are stronger for temporal sampling within the day).
- Because reducing pixel size and increasing the number of samples in the day both tend to increase P1, it may also be noted that a geostationary sounder could have a spatial resolution worse than a polar orbiter and still provide comparable or better values of P1. E.g. considering the 60 km FOR over London, the 20km GEO sensor provides higher N1 and P1 than 3 sun-synchronous orbits with 10 km pixel size. (However this is not true if 20 km FOR is required.)

P1 values for the UVN/SWIR species simulated here (NO_2, O_3, CO) are generally lower than for the TIR species (as a result of requiring daylight observations). There is therefore a greater margin for additional orbits to significantly increase P1:

- While cloud-free, daytime P1 values are generally substantially increased by adding GEO observations to polar combinations, this benefit is quite marginal once the modelled ability of retrieval schemes to account for cloud is accounted for. It should be that CH_4 has not been specifically simulated here, but it is assumed that the cloud-free sampling values are appropriate since even small amounts of cloud contamination are expected to limit the ability to meet user requirements. So for CH_4 there would be a particular benefit in P1 from adding geo observations to 9:30 + 1:30. However (i) the temporal sampling requirements for CH4 are relatively relaxed (threshold global sampling in 3 days) (ii) the focus for CH4 observations is not particularly over Europe but other regions of the globe not sampled by the GEO sounders relevant here.
- Sampling statistics for UVN/SWIR products depend on the length of the sun-lit day, and so depend more on time of year than the TIR products. For some of these species, GEO sampling seems to provide higher values of P1 in winter over London (e.g. CO), presumably by providing multiple observations which span the limited hours of daylight more optimally than the coarser temporal sampling of the polar orbiters.
- Of the explicitly simulated trace gases, NO2 generally has the lowest values of P1. However for London, the NSS and sun-synchronous combinations provide similar values of P1 to GEO and the NSS combination provides similar N1.
- Over Kampala the benefit of the NSS over the sun-synchronous combination is less marked, since the NSS combination is not optimised for such low latitudes. Kampala is not observed by the nominal GEO sounder, however results indicate that, particularly for the UVN/SWIR observations, GEO observations here would be particularly beneficial in raising P1 over the polar combinations. This is presumably related to the prevailing conditions of broken cloud and developing convection (for which sampling frequently helps find gaps), in combination with the extent to which the extreme edges of the polar swath are relied upon to give full daily longitude coverage in the tropics.
- In the Atlantic (as well as Cairo, Madrid) the single orbit values of P1 are so high that combinations add little to P1, only increasing N1. This is true except for the worst case FOR / pixel combination considered here (20km pixel, 20 km FOR) where it would appear that the NSS or GEO options add quite substantially to 3 sun-synchronous orbiters.

- Two simulations of tropospheric ozone are provided, based on the KNMI and RAL schemes. Of the two, the RAL results indicate a greater sensitivity to cloud contamination. In this case, the NSS combination provides best P1 values of over London. Improvements relative to the 9:30 and 13:30 combination are less pronounced for the KNMI results.

Aerosol simulations in task 5 are limited in a number of ways, notably that (a) the full spatial resolution of the 3MI sensor could not be simulated (b) the full dependence on observing conditions (geometric, surface reflection and aerosol load) of both the 3MI sensor and height-resolved retrievals from the A-band could only be handled in simplistic ways (c) aerosol will be sensitive to thin cloud which may not be well represented in the SEVIRI data. However the following points are worth noting:

- Of the species which have been simulated here, aerosol has the lower P1 and N1 values, representing the fact that the retrieval not only requires cloud free conditions, but is rather dependent upon observing geometry, hence statistics are generally worse than for simple cloud-free sampling.
- From the point of view of mission optimisation, clearly GEO orbit is not relevant to the 3MI concept which requires observations of the same point on the ground with multiple view angles. A geostationary platform provides better and more consistent sampling of the moderately high solar zenith angles which are favourable for A-band and single-view aerosol retrieval. This is particularly true of low latitude locations. This would imply that an A-band sounder of moderate resolution (i.e. coarser than the target 0.05nm resolution recommended in task 3) might more usefully be placed on a geostationary platform, in order to sample twice a day with favourable viewing conditions that might enable it to meet user-requirements relatively often (though this should be tested with more comprehensive simulations spanning the range of observing conditions).

Bearing the above considerations in mind the following conclusions are reached with respect to each of the missions scenarios proposed for Sentinel 4/5:

Geostationary and sun-synchronous polar orbit

This option is now clearly the baseline which will be implemented, with Sentinel 4 / 5 providing additional instrumentation along-side Meteosat Third Generation (MTG) and Post-EPS (in 9:30 orbit similar to Metop). Provided pixel sizes are compliant with the MRD, and given similar instrumentation on both platforms, the 9:30 would not add additional observations to those obtained from GEO, where the latter makes observations. Rather, the polar orbit complements GEO by providing observations globally whereas the GEO is focussed on the European sector, and by measuring species which are not measured by the GEO payload. In particular high-quality aerosol optical depth and composition provided by the 3MI sensor could only be provided from polar orbit, and the SWIR observations of CO and CH4 are not planned for the GEO platform at present. By sampling favourable high solar zenith angles more consistently however, the GEO may be a favoured platform for an oxygen A-band sounder to provide complementary information on the vertical distribution of aerosol.

Inclined non-sun-synchronous constellation

On the basis of these results, it is expected that a constellation of 3 (at most 4) NSS satellites, with inclination 55 degrees separated in orbit phase evenly through the day, would generally provide sampling which is comparable to that of GEO in the mid-latitudes. It would provide almost identical probabilities of obtaining a single observation in a day, but somewhat lower number of individual hours cloud-free within the day. The benefit over GEO would be that this sampling would be provided for all longitudes and include coverage of the tropics with slightly better sampling capabilities than an equivalent number of sun-synchronous orbits.

Sun-synchronous constellation

Combining observations from 9:30 and 13:30 sun-synchronous orbit leads to a substantial increase in the probability of obtaining compliant retrievals during a day, compared to 9:30 alone. Adding a further orbit with 17:30 local time further increases this probability (except for latitudes / months where this time is in darkness and sun-lit observations are needed). Adding 15:30 is less beneficial overall (though difference between adding 17:30 or 15:30 are slight). For pixel sizes around 10km and FOR 20 km or larger, 3 sun-synchronous polar orbits give probabilities of one observation per day which are close to the NSS combination or GEO, particularly for TIR products, though generally the number of samples within a day is substantially smaller for regions where the

NSS and GEO coverage is optimised. On the other-hand polar orbit provides far better sampling of the poles than the other platforms.

Given a realistic baseline for the Sentinel 4/5 that polar observations will be acquired from 9:30 and 13:30 orbit (Post-EPS and NPOESS), then it is clear from this analysis that the benefit of adding geostationary observations will be largely in terms of increasing the number of hourly samples acquired within the day, particularly for species for which sun-lit observations are required. GEO will not greatly increase the number of days on which a cloud-free observation is acquired. If this polar orbiter baseline is realised, then it seems sensible to optimise the GEO payload for species for which multiple samples during the day are a strong user requirement, e.g. NO2.

These conclusions on the relative benefit of combining observations from different orbits are based on the key assumption that both (i) the SEVIRI data-set used to simulate cloud occurrence and (ii) the LUTs which represent L2 retrieval sensitivity to cloud (and other parameters) are realistic. Work in task 4 has demonstrated the SEVIRI statistics to be robust cf MODIS, with the caveat that some thin cloud may be missed. The retrieval simulations underpinning the LUTs are also limited in the way they represent all the errors that may occur in the presence of cloud. For this reason, some caution should be exercised here: Both of these considerations will tend towards optimistic probabilities of any single observations being unaffected by cloud, and hence tend to reduce the apparent benefit of combining multiple observations.

7 Support to the Sentinel 4 and 5 Phase 0 and Phase A System Studies

7.1 Introduction

During the CAMELOT study system Phase 0 system studies have been conducted for the Sentinel 4 and 5 missions. These system studies have used draft versions of the MRD as a starting point. Questions raised on specific MRD issues that needed to be answered on the short term and could not wait on the final analyses of the study have been answered by the CAMELOT study team. In addition the support for the Phase 0 system studies, also the preparation of the Sentinel 4 Phase A ITT has been supported. Finally, studies have been performed for the Sentinel 5 Precursor missions, which was not in scope for the CAMELOT study.

In this chapter an overview will be given on the activities performed for Task 6 of the study. Results for the Sentinel 5 Precursor Orbit and temporal co-registration between the Sentinel 5 Precursor and a cloud imager are discussed in more detail.

7.2 Overview of the Activities of Task 6

Before the first progress meeting in July 2007, a list of 27 questions on the draft MRD was received from ESA. Of these 27 questions 5 were dealing with mission related requirements, 14 with the UVN on Sentinel 4 or Sentinel 5, 5 with the TIR on Sentinel 5 and 3 with the SWIR on Sentinel 5.
In November 2007 an additional set of 13 questions generated by the Phase 0 system studies was received from ESA. From this set of questions, 3 were dealing with mission related requirements, 6 with UVN and 4 with TIR requirements.

All these MRD questions have been addressed, although some had preliminary answers because further results were anticipated further on in the study.

During the CAMELOT progress meetings, action items have been raised on MRD related issues that had to be answered on short notice. In total more than 325 action items were addressed, for which some overlap with the MRD questions discussed above. Of these action items, 5 were dealing with mission related requirements, 18 with UVN, 4 with SWIR and 2 with TIR requirements.

In June 2008 an expert meeting on Sentinel was held at KNMI. In preparation for this meeting a list of 13 question was received from ESA. The study team has answered these questions. As an outcome of the meeting the CAMELOT team addressed 3 action items and 4 additional questions.

7.3 Orbit Possibilities for the Sentinel 5 Precursor

On request of ESA an assessment has been made on the orbit possibilities for the Sentinel 5 Precursor Mission, from the scientific and monitoring perspective. The precursor mission should serve as a gap-filler between the Envisat and the Post-EPS UVNS, with a target launch date of 2014. The minimum payload for the precursor mission is a UVNS instrument, which may be considered as a simple version of the LEO-UVNS instrument described in RD_1.

Although in this section it is assumed that the precursor mission will consist of only the UVNS instrument, it is noted that a combination of this instrument with a TIR sounder designed for ozone and carbon monoxide will have strong benefits. It is expected that synergistic use of these instruments will allow for improved retrievals of ozone and carbon monoxide profiles.

ESA has asked the CAMELOT study team for inputs on the possible orbits for the precursor mission. The purpose of this section is to recommend an orbit for the precursor mission based on considerations on synergistic observations and preferred time for operational usage of the data.

7.3.1 Synergistic Observation

The are two kinds of synergistic observations for the LEO-UVNS instrument:

I. Instruments that use the same observation technique and partly observe the same species. For example the spectral range of the LEO-UVNS partially overlaps with GOME-2 on Metop, resulting in the observation of the same species for this spectral range. Note that the spatial resolution and other instrument specifications can differ;
II. Instruments that provide observations on the same or other related target species in different spectral ranges or additional parameters, for example the VIIRS instrument NPP/NPOESS will provide additional information on clouds.

Synergistic observations of Type I are listed in Table 7-1 and for Type II in Table 7-2. Note that these tables are limited to the satellites flying in the period 2014-2019, thus Envisat and EOS Aura and Aqua are not considered in these tables.

Synergistic observations of Type I (measuring partially the same species) have the benefit that if the instruments fly in different orbits information on the diurnal cycle of atmospheric species can be observed. This has been shown for tropospheric NO_2 with the combination of OMI on Aura and SCIAMCHY on Envisat, RD_4. The Commission on Earth Observation Satellites (CEOS) has shown interest in such constellations. For the precursor mission the strongest constellation would be with the GOME-2 instrument on Metop. Since GOME-2 is in a morning orbit (local equator crossing time 9:30 AM), it would be best from the point of view of a Type I constellation to have the precursor in an afternoon orbit. In addition, the limb measurements of OMPS on NPP/NPOESS could provide additional information on the stratospheric ozone profile.

Table 7-1. UVNS Satellite instruments that will measure in period 2014-2019 that partially observe the same species.

Sensor	Satellite	Shared Species	Spatial Resolution	Dayside Local Equator Crossing time
GOME-2	Metop	Ozone, aerosols NO_2, HCHO, SO_2, O_2 etc..	40x80 km^2	9:30
OMPS	NPP/NPOESS	Ozone, aerosols	50x50 km^2	13:30

Table 7-2. Satellite instruments that will measure in period 2014-2019 that can provide additional information for UVNS retrievals

Sensor	Satellite	Additional Information	Spatial Resolution	Dayside Local Equator Crossing time
IASI	Metop	O_3 and CO profiles	18x18 km^2	9:30AM
AVHRR	Metop	Clouds	1x1 km^2	9:30AM
OLCI/SLSTR	GMES Sentinel 3	Clouds, aerosols	< 1x1 km^2	10:00AM
VIIRS	NPP/NPOESS	Clouds, aerosols	< 1x1 km^2	13:30PM 17:30PM
CRIS	NPP/NPOESS*	Ozone	< 20x20 km^2	13:30PM

*) It is not clear if ozone profile retrieval from CHRIS is possible.

Synergistic observations of Type II (additional information) can be used to improve the accuracy of the data products. For example, the retrieval of tropospheric trace gas products can be improved using the additional cloud information from imaging radiometers, which have a higher spatial resolution. Another example is the improved retrieval of ozone using the combined spectral information from the UV and TIR (IASI). Such combined retrievals are currently investigated, however their benefit has still to be proven using real data. It is noted that for the demonstration of combined ozone retrievals the combination GOME-2 and IASI can be used. For synergistic retrievals of Type II it is important that it can be assumed that the sensors observe the same atmospheric state on the spatial resolution of the UVNS instrument. This means that the time difference between the measurements of the precursor UVNS instrument and the synergistic observations should be of the order of a few minutes. Therefore, the UVNS instrument should either be on the same platform, or on a platform that is flying in formation with the platform from which the Type II synergistic observations are performed. Given the fact that the ozone synergistic retrieval can be demonstrated from GOME-2 and IASI, the strongest argument for Type II synergistic observations is for the additional information on aerosols and clouds, which can be achieved with Metop, Sentinel 3, or with NPOESS sensors.

7.3.2 Operational Data Use

In the CAMELOT study the time latency and delivery times for satellite data for air quality and UV forecasting applications have been investigated [RD_3]. From inquiries with responsible agencies in different European countries, two important times of the day for the operational applications have been identified:

- In the late afternoon decisions have to be made on possible legal actions for the next day. Such legal actions can include traffic or emission regularizations and/or formal warnings.
- In the morning information can be provided on the situation that is expected for the current day.

The decision making in the late afternoon is based on the current situation and meteorological forecast. Near real time satellite data could contribute to by providing information on the current situation. If late afternoon is assumed to be 17:00 hrs., and a 3 hours data latency is used, this means that the overpass should place before 14:00 hrs.

For providing information in the morning of a day, forecasts based on data assimilation available data and meteorological forecast can be used. Assuming that such forecasts have to be available around 7:00 in the morning, and that the processing will take several hours, the most recent UVNS observations are from the previous day, because these observations rely on daylight.

7.3.3 Long-Term Data Records

For monitoring of air quality and climate research, long-term data records are essential for deriving trends. For reactive gases, like NO_2 and tropospheric ozone, which have a strong diurnal cycle, the best way to build up consistent long-term data records is to measure at the same time of the day. For longer-lived species, such as ozone and carbon monoxide, it is less important to measure at the same time of the day. The UV-VIS observations of the precursor mission could either contribute to the long-term data record from GOME-SCIAMACHY-GOME-2 in the morning (equator crossing times between 9:30AM and 10:30AM), or to the afternoon record started by OMI (equator crossing time 13:35PM). The long-term data record of the morning orbit is ensured with the Metop GOME-2 series. The OMI data record of high spatial resolution trace gas observations (ozone, NO_2, SO_2, etc.) will be discontinued if the precursor mission is not flown in the afternoon orbit. The methane and carbon monoxide measurements will continue the SCIAMACHY measurements. As mentioned above, the overpass time for these gases is less important for deriving long-term trends.

7.3.4 Conclusions and Recommendations

Possible orbits for a precursor mission carrying a UVNS instrument in the time period 2014-2019 have been investigated on synergistic, operational, and data continuity aspects. The orbit is defined as a Sun synchronous orbits, for which the local equator crossing time at the dayside of the orbit is the free parameter.

The conclusions of this investigation are:

1. The UVNS precursor mission can be seen as a virtual constellation with the GOME-2 instrument on Metop. Since Metop is in a morning orbit (9:30AM crossing time), the precursor should be flown in an afternoon orbit. The UVNS also has strong links with IASI on Metop for ozone.
2. The UVNS instrument has synergies with imaging radiometers. To use the information on aerosols and clouds from the imaging radiometers, the UVNS instrument should fly in formation or should be integrated on the NPOESS, Metop, or Sentinel 3 missions.
3. For operational air quality applications the afternoon orbit is preferred because the near-real-time data available in the late afternoon can be used for the analysis of the current situation to support decision making for the next day. In addition, the afternoon orbit provides the latest observations from a UVNS instrument that can be used in forecasts that need to be available in the early morning of the next day.
4. Long-term data records are very important for monitoring and climate research applications. The afternoon orbit has the advantage that the OMI data record can be continued, whereas the morning long term data record is already secured with GOME-2.

Given the above-mentioned conclusions, we recommend to fly the UVNS precursor on a separate platform in formation with, or to integrate it on the NPOESS 13:30PM satellite.

7.3.4.1 References

RD_1 GMES Sentinels 4 and 5, Mission Requirements Document, Issue 1.0, 30 March 2007.

RD_2 Presentation of ESA at Camelot Progress Meeting, 17 January 2008.

RD_3 Camelot Task 2.2 Report, H. Elbern, October 2007.

RD_4 Boersma K. F., D. J. Jacob, H. J. Eskes, R. W. Pinder, J. Wang, R. J. van der A (2008), Intercomparison of SCIAMACHY and OMI tropospheric NO 2 columns: Observing the diurnal evolution of chemistry and emissions from space, J. Geophys. Res., 113, D16S26, doi:10.1029/2007JD008816.

7.4 Temporal Co-registration for Cloud Clearing

The retrieval of methane columns from the shortwave infrared spectral region is strongly affected by cloud contamination. To be able to measure methane with the required accuracy, cloud information is needed from other wavelength regions. As there is no cloud imager planned for the Sentinel 5 precursor (S5P) mission and information for the UVN spectrometer may be insufficient, it has been proposed to fly the S5P mission in formation with a satellite that has an instrument that can be used for accurate cloud-clearing.

In order to derive temporal co-registration requirements, ESA has requested from the CAMELOT study team to investigate the time difference between the measurement of the cloud mask and the measurement of methane. In this document we describe an investigation of this time difference using MSG SEVIRI data.

7.4.1 Method and Dataset

In this study we simulate measurements from two satellite sensors that measure at different times and study the effect of the time difference on the cloud clearing. The first measurement at t_0 is used for deriving a cloud mask and the second measurement at t_1 is for the retrieval of the trace gas (e.g. methane). Using this setup we study if the cloud mask derived on t_0 is still valid at t_1. As will be explained below, we classify ground pixel in 3 categories: clear, cloudy and cloud edge. Trace gas retrievals at t_1 will be performed on all pixels that are cloud free on t_0. If the cloud has changed in between t_0 and t_1, the pixel may no longer be cloud-free on t_1 and in this case cloud contamination will occur in the trace gas retrieval at t_1. The decision tree for determining if the trace gas retrieval will be successful or not is shown in Figure 7-1.

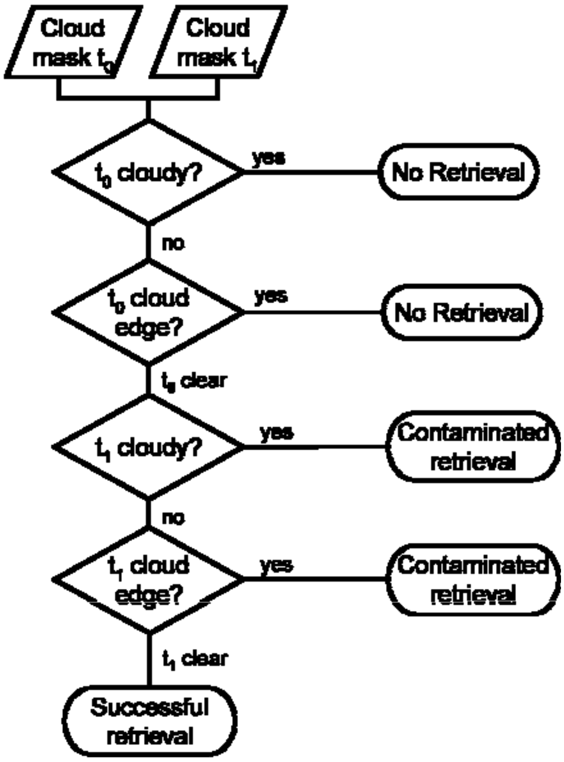


Figure 7-1. Decision tree to determine if a trace gas retrieval will be done at t_1, and if this retrieval will be successful or cloud contaminated.

The results in this document are based on the cloud properties retrievals developed by the EUMETSAT Climate SAF group [Roebeling et al, 2006]. The MSG SEVIRI instrument provides an image of the full disk every 15 minutes at several wavelengths from the visible to the thermal infrared, from which cloud information is derived. The spatial resolution of SEVIRI is approximately 3x3 km^2 at nadir. Over Europe the ground pixels increase strongly in the North-South direction due to the curvature of the Earth, which results in ground pixels of the order 3x6 km^2 over the mid-latitudes. In this study we are using SEVIRI data in the latitude range between 31 and 62 degrees North, and from -17 to 33 degrees East, see Figure 7-2.

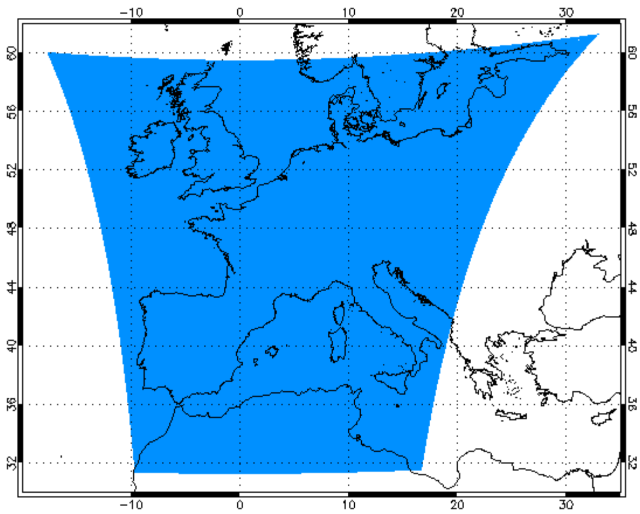


Figure 7-2. The geographical region used in this study.

As part of the retrieval described in Roebeling et al [2006], each SEVIRI ground pixel is quantified as cloud-free, containing water clouds or containing ice clouds, see Figure 7-3. In this study we treat both the ice and water clouds simply as cloudy pixels. For pixels to be identified as clear we require the pixel and its neighbouring pixels to be classified as cloud free. Therefore, we have introduced the cloud edge test, which ensures that the pixels on which methane retrievals would be performed do not suffer from cloud edge effects. It can also be used to avoid that in the time difference between t_0 and t_1 clouds can move close to, or into, a clear pixel. In the decision tree (Figure 7-1) we can use different edge constraints for the t_0 and the t_1 images. Also, different constraints can be used for the North-South and East-West directions, which were introduced because the ground pixels are rectangular over Europe. In the analysis different values were used for the cloud mask derived at t_0, but the t_1 edge tests constraint was always set to 1 neighbouring pixel in all directions. Figure 7-4 shows the constraints that have been used for the cloudmask at t_0. The different constraints will be referred to as case A (1 neighbour constraint), B (2 neighbour constraint) and C (4 neighbour in longitude and 2 neighbour in latitude constraint).

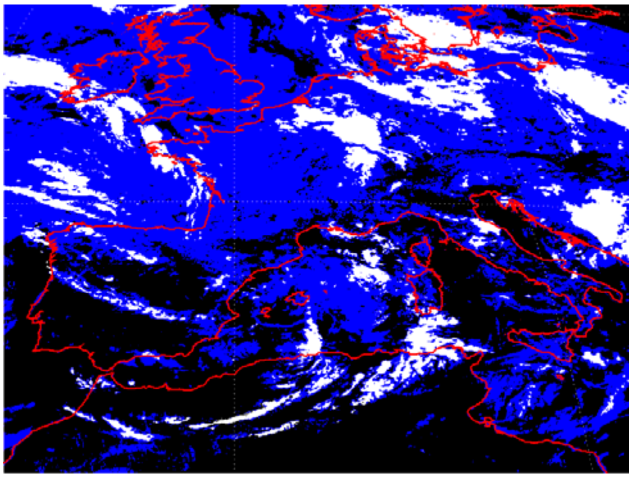


Figure 7-3. Example of the cloud classification by the CM-SAF algorithm. Black pixels are classified cloud-free, blue as water clouds and white as ice clouds.

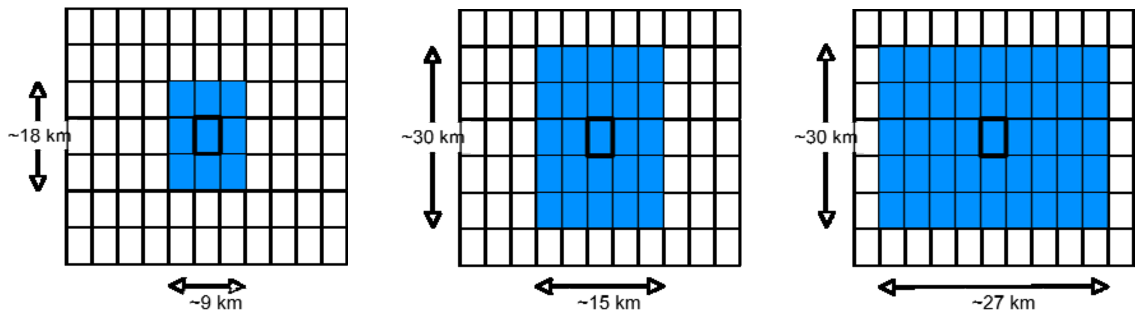


Figure 7-4. Schematic of the neighbouring ground pixels included in the edge test. The pixel that is test is the centre pixels in all figures. Left figure shows a test with 1 neighbour included in all directions (case A). The middle figure shows a test with 2 neighbours included in each direction (case B). The right figure shows a constraint with 4 neighbours in the East-West direction and 2 in the North-South direction (case C).

7.4.2 Results and Discussions

The results presented in this section are derived from SEVIRI cloud products for 2006 between 11:00 and 15:00 UTC. For each month of 2006, 6 days have been included in the analysis. For the cases A, B and C statistics are computed for all the pixels in the dataset. A pixel that contains valid data can be classified as:

- clear, meaning that the trace gas retrieval is assumed valid;
- cloudy meaning that no retrieval gas retrieval is applied; or
- cloud contaminated, meaning that the a retrieval is assumed to be applied, but the pixel contains a cloud or one of the neighbours contains a cloud.

The statistics for the Case A, B and C are presented in
Table 7-3,
Table 7-4, and
Table 7-5, respectively. In
Table 7-3 it can be seen that for Case A approximately 25% of the pixels is classified as clear when the time difference is 15 minutes. This number of pixels seems on the high end when compared to the study Krijger et. al, [2007]. Thus the cloud mask from SEVERI maybe less stringent than the one produced from MODIS. Therefore the number produced in this study should be evaluated in a relative way.

Table 7-3. Statistics for Case A.

t_1-t_0 [min]	Number of Pixels	Cloudy Pixels [%]	Clear Pixels [%]	Cloud Contaminated [%]
15	4.37E+08	72.31	25.18	2.516
30	4.25E+08	71.90	24.38	3.721
45	4.10E+08	71.43	23.88	4.691
60	3.95E+08	70.98	23.46	5.561

Table 7-4. Statistics for Case B.

t_1-t_0 [min]	Number of Pixels	Cloudy Pixels [%]	Clear Pixels [%]	Cloud Contaminated [%]
15	4.35E+08	77.32	21.77	0.9051
30	4.22E+08	76.96	21.31	1.731
45	4.08E+08	76.53	21.00	2.47
60	3.93E+08	76.12	20.71	3.167

Table 7-5. Statistics for Case C.

t_1-t_0 [min]	Number of Pixels	Cloudy Pixels [%]	Clear Pixels [%]	Cloud Contaminated [%]
15	4.33E+08	80.22	19.31	0.4718
30	4.20E+08	79.88	19.09	1.038
45	4.06E+08	79.48	18.91	1.606
60	3.91E+08	79.10	18.73	2.170

To quantify the effect of the time difference on the number of cloud contaminated pixels we express the cloud-contaminated pixels as percentage of the pixels for which a trace gas retrieval is assumed. The percentage of affected retrievals is calculated as:

Percentage affected = 100 ([cloud contaminated] / [[clear] + [cloud contaminated]]).

The percentage of affected retrievals is shown in Figure 7-5 as a function of the time difference between t_0 and t_1 for Case A, B and C. The lines in this figure are drawn through the origin, as the number of affected pixels at 0 time difference is per definition 0. As expected the percentage of affected pixels increases with increasing time difference. Also, the percentage decreases from Case A to Case C. If we apply a threshold value for the percentage of affected pixels of 2%, the time difference derived from Figure 7-5 ranges from less than 5 minutes for Case A to 15 minutes for Case C. For a 1% threshold the time differences range from 1 minute fro Case A to 7 minutes for Case C.

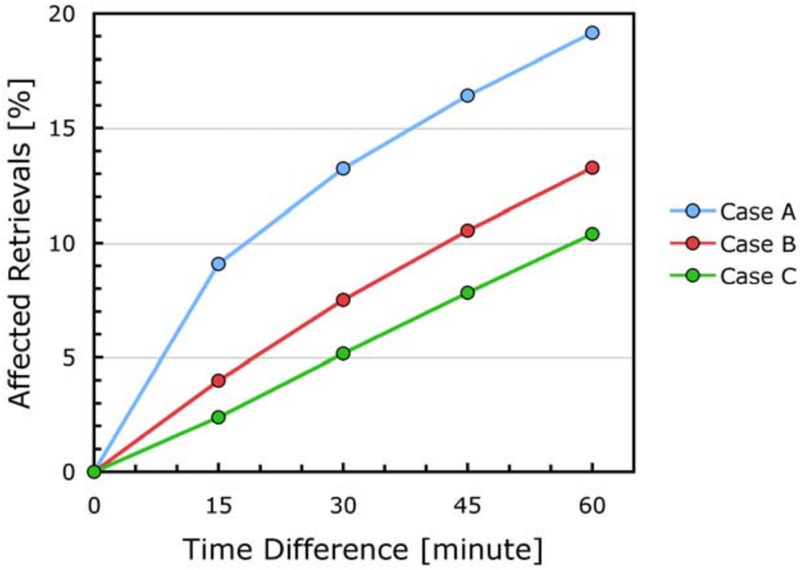


Figure 7-5. Percentage of affected trace gas retrievals as function of the time difference between t_0 and t_1 for Case A, B and C.

The constraints for cloud free pixels are stronger for Case B and C as compared to Case A. Therefore the number of cloud free pixels is lower for Case B and C, as can be seen in
Table 7-3,
Table 7-4, and
Table 7-5. The percentage of clear pixels is graphically displayed in Figure 7-6. This figure shows that the percentage of cloud free pixels decreases with approximately 5% from Case A to Case C. In a relative way, the decrease from Case A to Case C is 24%. It is noted that for a clear pixel the area without clouds is 5 times larger for Case C as compared to Case A, as can be seen in Figure 7-4.

In the MODIS study by Krijger et al. [2007] it was found that going from pixels with an area 9x18km^2 to 27x30 km^2 resulted in a decrease of clear pixels of 43%, which is much larger than the 24% found in this study. It is noted that the cloud edge test is different from the cloud test performed by Krijger et al., but the difference in decrease of clear pixels could also be the result of the different cloud clearing schemes.

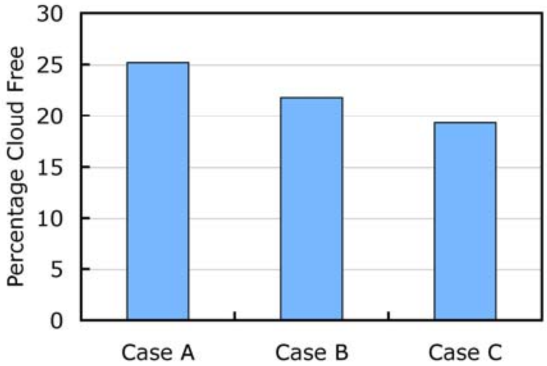


Figure 7-6. Percentage of cloud free pixels for Case A, B, and C.

7.4.3 Conclusions

We have presented statistical analysis of MSG SEVIRI data to study cloud contamination as function of the time difference between the cloud mask measurement and the trace gas measurement. This study has been performed for the Sentinel 5 Precursor measurements of methane, for which cloud information from another satellite may be used.

The results show that if 2% of the retrievals may be allowed to contain cloud contamination, the derived time difference between the satellites ranges from less than 5 to 15 minutes. If only 1% cloud contamination is allowed the time difference ranges from 1 to 7 minutes. The reported range is caused by different cloud mask constraints for the detection of cloud edges. When the constraints are stronger, the number of affected pixels decreases and the allowed time difference becomes larger. However, stronger constraints also result in less pixels passing the cloud tests and possibly marking clear pixels as cloudy. From the weakest to the strongest constraints used in this study, the number of clear pixels decreased by 20%. A recent study using MODIS data reported a 43% decrease with increasing region of interested. This larger difference should be further investigated.

The results in this study are limited to MSG data over Europe, which have a typical spatial resolution of 3x6 km^2. The Sentinel 5 Precursor SWIR measurements are expected to have a spatial resolution of $10x10km^2$ at nadir, and the cloud mask from for example VIIRS on NPOESS less than 1x1 km^2. The improved spatial resolution of the cloud mask will drastically increase the information on clouds. It is expected that this information can be used to optimize the cloud clearing procedure.

8 Concluding Remarks

The CAMELOT study has resulted in detailed results in support of the Sentinel 4 and 5 missions. In this report the high-level results are presented and more detailed results can be found in the individual task reports. For the assessment of the user requirements the MRD Tables B1, B2 and C1, addressing air quality protocol monitoring, near-real-time and climate protocol monitoring applications, were in scope for the study. The analyses performed in the CAMELOT study have led to the following conclusions and recommendations.

Within the CAMELOT, study datasets of four-dimensional fields of aerosol and trace gases have been produced using state-of-the-art chemistry-transport and climate models. The spatial-temporal variability in these is larger than the variability due to the different IPCC emission scenarios. Therefore, the selected profiles, which span a wide range of trace gas and aerosol concentrations, are representative for the current as well the future variability in trace gas and aerosol concentrations.

The CAMELOT study has considered auxiliary variables, which need to be measured in order to deliver required output product quality for the Sentinel 4/5 system. These include auxiliary information required for product development in the ground segment, for quality control/quality assurance (QA/QC) and for the application areas of air quality and climate.

For product development, the main new finding was that the scattering path for SWIR measurements of CH_4 needed to be determined using the O_2 A-band, but also by including CO_2 measurements at 1.6 µm (the “proxy” method); this was subsequently confirmed by retrieval simulations in the study. Cloud and aerosol determination was also recognised to be important but this was expected in the study. Other new requirements noted were for surface albedo/emissivity maps and digital elevation models in the ground segment as well as meteorological analysis/forecast data. If vertical column densities are to be provided, then for NO_2, for example, a chemical-transport model or its outputs needs to be included in the ground segment.

For QA/QC, validation requirements are maturing at a reasonable rate. There are, however, some critical issues, which include ensuring the accuracy and consistency of air quality measurements in the urban areas and for greenhouse gases for climate. For air quality, the key issue is a representative, long-term operational network for NO_2 with verifiable performance.

A user survey and published literature suggested that it is desirable for a satellite product estimating the photolysis rates for NO_2 to be produced. The survey and published air quality reports showed the requirement for daily image data of the MODIS form. Other desirable aspects included requirements for aerosol with dust separation, fire maps, land cover and land surface temperature. Sentinel 3 data are recognised to be an important future source for these data sets and support should be given to production of the appropriate data sets for atmosphere applications.

Applications in the climate area emphasized the importance of producing, as an output, mean dry mole fraction or mean dry air mixing ratio is standard – the product is often denoted as XGas so XCO_2 or XCH_4. The corresponding auxiliary data requirements for methane are for O_2 and CO_2 columns (surface pressure) for normalisation to mean dry air mixing ratios; this is similar to the scattering path consideration noted previously. For auxiliary data for greenhouse gas inverse modelling and for assimilation of greenhouse gases, the most important parameters are fire (burned area), land cover maps, vegetation intensity indication for land; ocean colour and sea surface temperature for the ocean; atmospheric chemistry observations which constrain OH. Note that CO measurements are required for CH_4 inverse modelling since CH_4 and CO are inter-linked as per the CAPACITY study findings.

For delivery requirements, delivery times for satellite data were divided into NWP/UV forecast applications, and air quality forecast and monitoring. For NWP/UV forecast applications, an estimated 4 hours acceptable delay time for NWP purposes is sufficient. For air quality forecast and monitoring, at least a delivery time of 3 hours maximum is required. In the case of ozone and tropospheric aerosols, somewhat relaxed delivery times may be acceptable, with ozone estimated 5 hours and aerosol about 8 hours. In any case, photochemically highly reactive species as NO_2 impose the time limiting conditions. As concerned the hour of delivery, no clear indication of preference could be gained from users. However, with sensors operating in the UV-VIS range, late afternoon delivery is a preferable choice.

In the CAMELOT study, the Level 1B requirements for the foreseen instruments on the Sentinel 4 and 5 have been derived using retrieval simulations as the most important tool. It is recommended to change the MRD requirements according to the recommendations given in section 4 of this document and the underlying Task 3 task reports.

As compared to the values of the MRD version at the start of the study, the main change in the UVN spectrometer was an increase in signal-to-noise in the visible channel, whereas other requirements were refined or confirmed. The Sentinel 5 TIR system concept was fully studied in CAMELOT. Strongly revised recommendations in comparison with MRD version 2.0 are provided based on the simulation results of CAMELOT, the lessons learned from IASI and the homogenisation between Sentinel 5 and Post-EPS MRD. For the SWIR spectrometer it is recommended to revise several Level 1B requirements. An important recommendation for the SWIR spectrometer is to increase the priority of the 1.6 µm band to priority 1, in order to enable three band retrievals for methane. The 1.6 µm band may also be used for the retrieval of CO_2, for which the retrieval simulations showed good performance with some limitations for cirrus and aerosol cases. The GOSAT mission should confirm these findings for the retrieval of CO_2.

The user requirements for sulphur dioxide and formaldehyde will not be met with a realistic UVN spectrometer. These species need a very high signal-to-noise ratio to be able to observe background concentrations in individual measurements. For sulphur dioxide, volcanic plumes are an exception because these plumes have typically high concentrations and the sensitivity of the measurement increases with altitude. Although most measurements of formaldehyde and sulphur dioxide do not meet the user requirements for individual measurements, they will be used after temporal and/or spatial averaging to improve the emission inventories, which are essential input for air quality and chemistry-transport models.

It is recommended to review some of the user requirements given in the MRD. The consensus of the CAMELOT consortium was that the user requirements for the total and tropospheric column of CO are too relaxed. For formaldehyde and sulphur dioxide the requirement were seen as too strict. Also, it is recommended to review the user requirements for HNO_3 and PAN. It may be considered to specify the user requirement for CO_2 in more detail. In addition, it should be considered to add user requirements for species including ammonia and glyoxal, for which satellite based measurements are demonstrated.

It is recommended for the Sentinel 5 mission to include the UV-TIR and SWIR-TIR spectral ranges needed for the combined retrievals of ozone and carbon monoxide, which offer theoretically significant improvements in the troposphere and the PBL. For that purpose, the spatial co-alignment between the UV and TIR, and the SWIR and the TIR ground pixels should be of the order of a few kilometres, matching the expected ozone and carbon monoxide tropospheric variability. The temporal requirements are of the order of a few minutes. Therefore, it is recommended to put the UV, SWIR and TIR spectrometers on the same satellite platform.

It is recommended to develop the combined retrievals for real data using IASI and GOME-2 data and TES or AIRS and OMI data. The retrievals on data from these instruments should demonstrate the feasibility of ozone combined retrievals for monitoring purposes.

In support for the combined UV-TIR ozone retrievals and SWIR-TIR carbon monoxide retrievals, consistent spectroscopic laboratory measurements for these wavelength bands are needed at the relevant atmospheric temperatures and pressures.

The sensitivity of UVN observations to boundary layer ozone is low. In combination with the relatively small contribution of the boundary layers ozone to the tropospheric column, polluted boundary layers can only be observed for very strong pollution events, in combination with high boundary layers. The diurnal variations in ozone are predominantly confined to the boundary layer. Therefore, the observation of the diurnal variation in ozone by the Sentinel 4 UVN will be limited to specific cases for large Mediterranean cities during pollution events, for which high ozone concentrations and thick boundary layers can occur.

To measure the aerosol optical thickness up to the user requirements and to derive aerosol type information, a directional polarization instrument should be added to the Sentinel 5. The UVN instrument alone cannot make the aerosol observations that meet the user requirements. The directional polarization instrument will measure radiance and the polarization at selected wavelength bands for the UV to the SWIR in multiple viewing directions. Such an instrument has strong synergy with the NIR channel of the UVN instrument, because of the aerosol height information in the O_2-A band. This synergy can be exploited if the directional polarization instrument and the UVN observations are co-located, which can be achieved by putting them on the same platform. Also, the directional polarization instrument will benefit from co-location with the cloud imager.

It is recommended to fly the Sentinel 5 Precursor mission in an afternoon Sun synchronous orbit, for the following reasons:

1. The UVN instrument in the afternoon orbit and the GOME-2 instrument in the morning orbit can provide information on the diurnal cycle of trace gases;
2. The UVN in the afternoon orbit will continue the data record of OMI, whereas GOME-2 continues the record of the morning orbits from GOME and SCIAMACHY.
3. For air quality forecasts the UVN observations are needed in the afternoon.

Because the methane retrievals from the SWIR need very accurate cloud clearing, it is recommended to fly the Sentinel 5 Precursor mission within 10 minutes of the NPP/NPOESS mission, to allow the use of the VIIRS instrument for this purpose.

Bearing the cloud-free and L2 sampling statistics for various orbit combinations, together with other constraints on the mission, the following conclusions were reached with respect to each of the missions scenarios proposed for Sentinel 4 and 5:

- Geostationary and sun-synchronous polar orbit combination is now clearly the baseline which will be implemented, with Sentinel 4 / 5 providing additional instrumentation along-side Meteosat Third Generation (MTG) and Post-EPS (in 9:30 orbit similar to Metop). Provided pixel sizes are compliant with the MRD, the 9:30 orbit would not add significant additional sampling to that obtained from GEO, in the region where the latter makes observations (i.e. the European sector). Rather, the polar orbit will complement GEO by providing observations globally and by measuring species, which are not possible with a GEO payload.

- A non-sun-synchronous constellation consisting of 3 satellites, with inclination 55 degrees separated in orbit phase evenly through the day, would generally provide sampling which is comparable to that of GEO in the mid-latitudes. It would provide almost identical probabilities of obtaining a single observation in a day, and only slightly fewer individual hourly samples within the day. The benefit over GEO would be that this sampling would be provided for all longitudes and include coverage of the tropics with slightly better sampling capabilities than an equivalent number of sun-synchronous orbits.

- Forming a Sun-synchronous constellation by combining observations from 9:30 and 13:30 sun-synchronous orbit leads to a substantial increase in the probability of obtaining compliant retrievals during a day, compared to 9:30 alone. Adding a further orbit with 15:30 *or* 17:30 local time further increases this probability though little would be further gained by adding both. For pixel sizes around 10 km and a field of regard of 20 km or larger, 3 sun-synchronous polar orbits give probabilities of one observation per day which are close to the NSS combination or GEO, particularly for TIR products, though generally the number of samples within a day is substantially smaller for regions where the NSS and GEO coverage is optimised. (However it is clear that sun-synchronous orbit provides far better sampling of the poles than the other options.)

- Given a realistic baseline for the Sentinel 4/5 that polar observations will be acquired from 9:30 and 13:30 orbit (Post-EPS and NPOESS), then it is clear from this analysis that the benefit of adding geostationary observations will be largely in terms of increasing the number of hourly samples acquired within the day, particularly for species for which sun-lit observations are required. GEO will not greatly increase the number of days on which a cloud-free observation is acquired. If this polar orbiter baseline is realised, then it seems sensible to optimise the GEO payload for species for which multiple samples during the day are a strong user requirement.

It is essential to have support of scientists throughout the design and build of the Sentinel 4, Sentinel 5, and Sentinel 5 precursor instruments. Using retrieval simulations and/or experience, scientists can assess the effects of instrument trade-offs, such as specific features of the Level 1B data on the Level 2 data, or when certain requirements are difficult to meet.

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List of Acronyms

AOT	Aerosol Optical Thickness
AQ	Air Quality
CAMELOT	Chemistry of the Atmosphere Mission concEpts and sentineL Observations Techniques
CAPACITY	Composition of the Atmosphere; Progress to Applications in the User Community
CHIMERE	A multi-scale chemistry-transport model of IPSL for air quality forecasting and simulations (http://euler.lmd.polytechnique.fr/CHIMERE/)
CrIS	Cross track Infrared Sounder (instrument on board NPP/NPOESS)
CLRTAP	Convention on Long-Range Transboundary Air Pollution
DOAS	Differential Optical Absorption Spectroscopy
DU	Dobson Unit
EC	European Commission
ECMWF	European Centre for Medium-range Weather Forecasts
Envisat	ESA Environmental Satellite
EO	Earth Observation
EOS-Aura	Earth Observing Systems Aura Mission
EPS	EUMETSAT Polar System
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
G	Goal; desirable value for a requirement
GAS	GMES Atmospheric Service
GEMS	Global and regional Earth-system (Atmosphere) Monitoring using Satellite and in-situ data; EU Project concluded in May 2009.
GEO	Geostationary Earth Orbit
GMES	Global Monitoring for Environment and Security
GOME	The Global Ozone Monitoring Experiment
GOSAT	Greenhouse gases Observing SATellite
IASI	Infrared Atmospheric Sounding Interferometer
IFOV	Instantaneous Field of View
IGBP	International Geosphere-Biosphere Programme
IPCC	Intergovernmental Panel on Climate Change
IR	InfraRed
LEO	Low Earth Orbit
Level 1B data	Callibrated and geolocated (ir)radiance data
Level 2 data	Data of geophysical parameters (e.g. ozone layer) on the satellite’s measurement grid
MACC	Modelling Atmospheric Composition and Climate; EU project, follow-on projects for GEMS and PROMOTE
Max-DOAS	Multi-Axis Differential Optical Absorption Spectroscopy
Meteosat	Geostationary meteorological operational satellites of EUMETSAT
Metop	Meteorological operational satellites of the EUMETSAT Polar System (EPS)
MRD	Mission Requirements Document for GMES Sentinels 4 and 5, Issue 1, draft 3
MSG/MTG	Meteosat Second Generation/Meteosat Third Generation

NDACC	Network for the Detection of Atmospheric Composition Change
NIR	Near-InfraRed
NPOESS	Polar Orbiting Earth Operational Environmental Satellite
NPP	NPOESS Preparatory Project
NRT	Near Real Time
NSS	Non Sun Synchrnous; inclined orbit
NWP	Numerical Weather Prediction
OCLI	Ocean Land Colour Instrument
OMI	Ozone Monitoring Instrument (http://www.knmi.nl/omi)
OMPS	Ozone Mapping and Profiler Suite (instrument on board NPOESS)
PROMOTE	PROtocol MoniToring for the GMES Service Element: Atmosphere; ESA funded project
Ppb	parts per billion
Ppbv	parts per billion by volume
Pptv	parts per trillion by volume
SNR	Signal to Noise Ratio
S/W	Software
SCIAMACHY	Scanning Imaging Absorption SpectroMeter for Atmospheric CarograpHY
SLSTR	Sea and Land Surface Temperature Radiometer
SWIR	Short Wave InfraRed
T	Threshold; value required to meet the user requirements
TBA	To Be Added
TBC	To Be Confirmed
TBD	To Be Determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal InfraRed
TM	Tracer Model (versions TM3, TM4 and TM5 of the KNMI atmospheric chemistry transport model) (http://www.knmi.nl/~velthove/tm.html)
UV	Ultraviolet
VIIRS	Visible/Infrared Imager Radiometer Suite
VIS	Visible