CAMELOT
Executive Summary

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ESA STUDY CONTRACT REPORT

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ABSTRACT

This report is the executive summary of the 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 missions. This report presents the main conclusions and recommendations of this study, regarding the Sentinel 4 and 5 Level 1B requirements and the mission scenario's.

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1 Introduction

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:

- Task 1: 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.

2 Geophysical Scenario’s

The CAMELOT study required geophysical scenarios of the atmosphere and surface reflectance 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.

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. Therefore, the set of requirements made it necessary to use more than one model for the construction of the scenarios.

Scenario requirements for 2015 have been formulated in consensus with the CAMELOT partners and are documented in TN-CAM-FMI-006. The selected locations are presented in Table 2-1 and shown in the map of Figure 2-1. These scenarios are based on IPCC and recent developments as explained in RP-CAM-FMI-030.

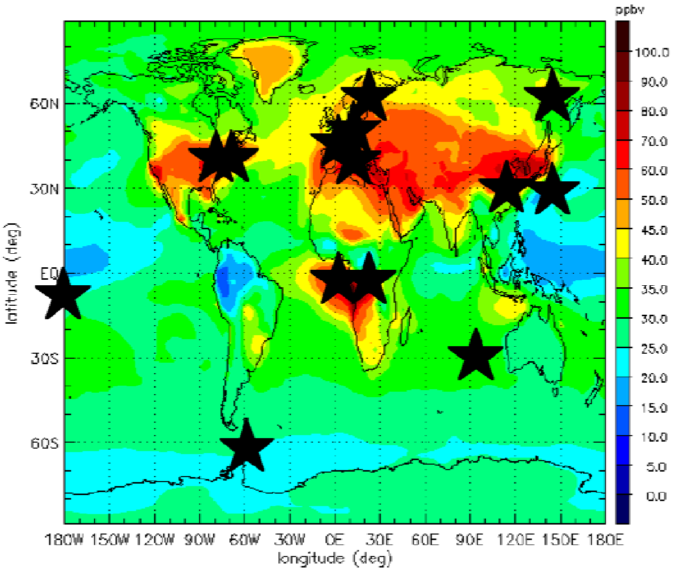

Figure 2-1. The geographic spread of the 14 selected locations. The underlying map shows the surface ozone concentrations (in ppbv) for June 2000 simulated using TM4.

Table 2-1. 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	Longitude	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

2.1 Description of the Models

Three models were used to generate the CAMELOT database. The coupled atmosphere-ocean general circulation climate model of the Max Planck Institute for Meteorology (MPI-M) 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 necessary elements used for the aerosol scenario production were: a size resolving model of aerosol microphysics, a model for natural primary aerosol emissions, and scenarios for primary anthropogenic aerosol emissions for year 2015 in accordance with the IPCC storylines A2, A1B and B1. ECHAM5 is coupled with the Hamburg Aerosol Model HAM (Stier *et al.*, 2005).

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.

CHIMERE is a three-dimensional Eulerian chemistry-transport model. For the CAMELOT study, a continental configuration over Western Europe with a horizontal resolution of 0.5 × 0.5 degrees was used with a time step of 10 minutes and hourly model output. A simulation for June 2006 was provided for CAMELOT.
The data provided by these models are summarized in Table 2-2.

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

MODEL	ECHAM5-HAM	TM4	CHIMERE
Time resolution	6 hours	Monthly average	1 hour
Spatial resolution	T42 (approx. 300 km at equator)	3 × 2 (lon × lat) degrees	13 × 13 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

2.2 Scenarios

The future climate scenarios provided by the Intergovernmental Panel on Climate Change (IPCC) have been utilized to provide realistic climate scenarios. They are based on hypothetical scenarios of CO_2 and other greenhouse gas emissions under different socio-economic assumptions. For CAMELOT were considered 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).

Each ECHAM5-HAM experiment was started from 1 Jan 2010 with its own boundary conditions until 31 Dec 2013 to allow the climate model system to spin down to the attractor limited by the provided AR4 boundary conditions. From 1 Jan 2014 each experiment continued with the estimated emissions for 2015 following the A2, A1B and B1 scenarios. The control experiment continued with the standard AEROCOM2000 emissions. Experiments were stopped 31 Dec 2015.

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). For CAMELOT the intermediate 'CLE (Current Legislation)' scenario was used. The CLE scenario is based on the moderate IPCC SRES B2 energy scenario. 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.

Information on the surface reflectance was provided as surface albedo data from various sources, with wavelengths ranging from the ultraviolet (~300 nm) to the thermal infrared (~15 µm).

3 Complementary Observations and Delivery Requirements

Task 2 of 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.

3.1 Geophysical Observation Requirements for Auxiliary Data

The area of auxiliary data is quite extensive for the Sentinel 4 and 5 missions, as for any atmosphere mission addressing a range of trace gases. Auxiliary requirements for the following areas can be distinguished:

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 (QC) and quality assurance (QA)** of operational products (validation for operational systems).
3. Auxiliary data required for key, higher level, **application areas** in the core and downstream services, including data assimilation systems (Level 4 products).

3.2 Auxiliary Data for Data Processing Systems

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 retrievals. The analyses presented here are based on questionnaires, literature surveys and the analyses of Task 3 and 4.

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*

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

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.

Ground segment requirements are for the following data sets: meteorological forecast temperature/ humidity/surface pressure; digital elevation databases; surface albedo/emissvity databases; climatologies of target gases (and their contaminants); spectroscopic databases. In addition, chemical-transport models would be required for specific Level 2 products, e.g. for the shapes of tropospheric profiles and knowledge of the stratospheric burdens of some species.

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.

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.

3.3 Auxiliary data for Quality Control and Quality Assurance

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, NDACC, 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 which is considered briefly below.

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 larger 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:

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.

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

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.

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 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 and hence long-term inter-calibrated measurements are required.

3.4 Auxiliary data for Air Quality and Climate Applications

The intended applications for the missions considered in the CAMELOT study can be broken down into air quality and climate. In the study it was 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 this restriction, it is worth noting that there are certainly auxiliary data sets, available from other Sentinels, which will support the application areas.

3.4.1 Air Quality

The air quality area is complicated as there are a number of ways in which satellite data can be used in the air quality problem and there also 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 can also 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.

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.

Regional modelling and local/regional air quality 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 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.

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.

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.

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. 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.

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.

3.4.2 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. 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.

In **inverse modelling of emissions**, 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 O_2 columns (thus also reducing photon path errors) or through the use of surface pressure (see also Section 3.2).
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 3.4.1).

In terms of **data assimilation for climate**, 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.

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.

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

3.5 Delivery Times for Air Quality Information

Task 2.2 focussed on requirements for data delivery times for the Sentinel 4 and 5 ground segment. Depending on individual applications, the question of delivery time can be understood in two different ways: (1) delivery as fast as possible, independent of time of day, and (2) 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 and beyond the scope of the study.

Four different kinds of users may be identified to be reliant on fast data delivery of data envisaged for the 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.

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;
- 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

In the CAMELOT retrieval simulations have been carried out to derive Level 1B requirements from the Level 2 requirements and to assess the expected performance of the Sentinel 4 and 5 missions. In Table 4-1 the species are listed that have been studied within CAMELOT. As indicated in this table, for some of the species, like ozone and carbon monoxide, more than one spectral range has been studied. In addition to trade-off studies for these species, also the synergy between the observations has been investigated, for example by performing retrievals that combine the information from two spectral ranges.

The comparison between the expected performance of the Sentinel 4 and 5 instruments for the user requirements of the MRD is given in Table 4-2 and Table 4-3. The interpretation of the user requirements is that they have to be met on individual observations, thus without temporal or spatial averaging. Furthermore, the accuracies given for the user requirements include both random and systematic errors. The MRD contains per species and application several requirements. Not all these requirements have to be met for each species. Table 4-2 presents the comparison of the expected performance versus the threshold user requirements. These threshold user requirements have been selected from the MRD Level 2 requirements and represent for each species the requirements on the total and/or the tropospheric columns. The more demanding Level 2 requirements are compared to user requirements in Table 4-3. As can be seen in Table 4-2 most of the threshold Level 2 requirements are expected to be met with the observations recommended by the CAMELOT study, except for sulphur dioxide (SO_2), formaldehyde (CH_2O), N_2O_5 and PAN. It is noted that, although the user requirements for these species will probably not be met, these products are still useful after spatial and temporal averaging for deriving long term trends and to constrain emissions and sinks for chemistry transport models. For several species, including carbon monoxide, sulphur dioxide, formaldehyde, nitric oxide, N_2O_5 and PAN it is recommended to review the user requirements.

Table 4-1. Observational principles for the 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		
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

For carbon dioxide 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. Most of the goal requirements are not met (Table 4-3), because the vertical resolution for most of these requirements is much higher (1-3 km in many cases) than can be achieved from spaceborne observations. The diurnal information on ozone from UV observations will be limited to large cities in the Mediterranean region and strong pollution events in the summer. This limitation is caused by the decreasing sensitivity for ozone in the boundary layer, which cannot be improved by more stringent Level 1B requirements.

Table 4-2. Assessment of the expected performance versus the threshold user requirements. Green colours 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 4-3. Assessment of the expected performance versus the goal user requirements. Green colours 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	--	

In the CAMELOT study combined retrievals have studied for ozone using UV and TIR observations, and for CO using SWIR and TIR observations. 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 and not with real instruments. Real instruments are 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, TES/OMI) are expected to show if the theoretical gain of combined UV-TIR ozone retrieval can be achieved in practice. A prerequisite for the success of this combined retrieval is a consistent set of spectroscopic data for the UV and the TIR, which is currently not available.

The results for the combined SWIR-TIR retrieval of carbon monoxide also shows enhanced information in the troposphere. With the combined retrievals carbon monoxide in the lower troposphere, in which the emissions of take place, can be distinguished from carbon monoxide in free troposphere, which I dominated by long-range transport. Unlike the situation for ozone, there are currently no co-located observations to develop the combined on real instruments.

Although no simulations have been performed for combined retrieval of aerosol from directional polarization observations, in combination with aerosol information from absorption bands, there is a strong synergy between these measurements. The directional polarization observations will deliver column-integrated quantities, like the aerosol optical thickness and the single scattering albedo, the absorption bands in the NIR and SWIR contain information on the vertical aerosol distribution.

To enable the combined retrieval, the observations (i.e. UV-TIR for ozone, SWIR-TIR for carbon monoxide, and directional polarization-NIR) should be collocated in space and time. Because of the importance of clouds in the lower troposphere, these measurements have to be collocated within 1-2 minutes.

4.1 Sentinel 5 Level 1B Requirements

The Sentinel 5 is a mission in a Sun synchronous low Earth orbit. The Level 1B requirements for the following nadir viewing Sentinel 5 instruments have been studied in CAMELOT:

- UV-VIS-NIR (UVN) spectrometer;
- TIR spectrometer;
- SWIR spectrometer;
- Directional Polarization Imager (DPI).

In addition to these instruments, the assumption is made that a cloud imager with a higher spatial resolution and sampling with channels in the VIS-NIR and TIR is available making temporal collocated measurements. Below the high-level Level 1B requirements of the instruments studied are given.
In the following section recommendations for the main characteristics for these instruments are summarized.

4.1.1 UVN spectrometer

The Sentinel 5 UVN spectrometer will be used to measure the concentration of the following tropospheric trace gases: ozone, nitrogen dioxide, sulphur dioxide, formaldehyde, water vapour and brome oxide. In addition it provides information on aerosols and clouds.

The Sentinel 5 UVN spectrometer 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. The recommended characteristics of the spectral bands for the Sentinel 5 UVN spectrometer are given in Table 4-4.

Table 4-4. Recommended characteristics for the spectral bands for the Sentinel 5 UVN. Goal requirements are given in parenthesis.

Band ID	Spatial Resolution [km]	Spetral Range [nm]	Spectral Resolution [nm]	Sampling Ratio	SNR[1,2,3]	Driving species
UV1	≤50 (≤15)	270-310	≤1.0	≥3	≥100 @ 270 nm	O_3
UV2	≤15 (≤5)	300-380	≤0.5	≥3	≥1000 @ 310 (320) nm	O_3 (SO_2, CH_2O)
VIS	≤15 (≤5)	360-500	≤0.5	≥3	≥1500 @ 420 nm	NO_2
NIR	≤15 (≤5)	710[4]-775	≤0.4 (0.05)	≥3	≥500 @ 755 nm [5]	Clouds (Aerosol)

1) *The SNR is given per spectral sample for a spectral sampling ratio of 3.*
2) *The SNR is given for the reference spectrum delivered by the CAMELOT study*
3) *The SNR is given at one wavelength. The shot noise model is assumed to calculate the SNR at other wavelengths.*
4) *The start wavelength for the NIR is driven by water vapour; the O_2-A band starts at 755 nm.*
5) *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.*

Table 4-5. Spectral requirements and NeDT values for Sentinel 5 TIR spectrometer. 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*

4.1.2 TIR spectrometer

The TIR spectrometer will be used to measure tropospheric concentrations of ozone, carbon monoxide, methane, nitric acid, PN and water vapour. IASI experience shows that also other minor atmospheric constituents like ammonia and methanol can be measured, provided that the spectral range covers these gases.
The TIR sounder here will make observations in the nadir geometry 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 instrument should allow for twice daily coverage of the whole Earth. The spatial resolution is 12 × 12 km^2 with a goal value of 5 × 5 km^2 .

During the project, the decision to the merge Sentinel 5 and Post-EPS programmes has significantly changed the perspective. 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*

4.1.3 SWIR spectrometer

The SWIR is used to measure the concentration of the trace gases carbon monoxide, methane and carbon dioxide. In addition the SWIR contains information on the vertical profile of aerosols and clouds and the water vapour column. Within the CAMELOT study, carbon monoxide and methane were the main drivers for the SWIR channel. Carbon dioxide was given lower priority, which follows the recommendation from the GMES Atmospheric Services (GAS) group.
The Sentinel 5 SWIR spectrometer 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. The recommended characteristics of the spectral bands for the Sentinel 5 UVN spectrometer are given in Table 4-6.
An important trade-off for the Sentinel 5 SWIR spectrometer is the priority of the spectral bands. Both carbon monoxide and methane can be retrieved from the SWIR-3 spectral band, in combination with the cloud information from the UVN NIR channel and the cloud imager. However, the CAMELOT simulations show that use in addition to these bands also the SWIR-1 band are significantly less sensitive to inference of cirrus clouds and aerosols. Therefore, it is recommended to increase the priority of this band as compared to the MRD.

Table 4-6. Recommended characteristics for the spectral bands for the Sentinel 5 SWIR spectrometer.

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

1) *The SNR is given per spectral sample for a spectral sampling ratio of 2.5.*
2) *The SNR for SWIR-1 and SWIR-3 are given for the reference spectra delivered by CAMELOT*
3) *The aerosol height retrievals from the SWIR 2 band are not considered mature. The preffered 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.*

4.1.4 Directional Polarization Imager

The directional polarization imager is focused on the requirements for aerosols. Analysis performed in CAMELOT show that to meet the user requirements for aerosols on both the aerosol optical thickness and aerosol type, described as a combination of the aerosol size distribution and the refractive index, such an instrument is essential. The version of the MRD that was used as a starting point of the CAMELOT study did not include requirements for multi-viewing and polarization observations. The Level 1B requirements for the directional polarization imager are based on limited analyses, using the 3MI instrument concept under study for EUMETSAT Post-EPS as input.

The DPI should measure total reflectance and Stokes fractions $q = Q/I$ and $u = U/I$ at multiple viewing angles in the spectral channels listed in Table 4-7 with polarization in a subset of these spectral channels. The DPI should observe a ground pixel under at least 10 viewing angles in the range -50^{o} to 50^{o}, with a spatial resolution of threshold 2 and goal 1 km. The user requirements on the relevant aerosol parameters are met under most circumstances for relative azimuth angles less than 40^{o} (defined such that a relative azimuth angle of 0^{o} corresponds to the principal plane). It is noted that these geometrical requirements can only be met from a LEO orbit.

Table 4-7. Definition of the bands for the DPI.

Band ID	Central Wavelength [nm]	FWHM [nm]	Polarization
1	354	20	
2	388	20	x
3	443	20	x
4	490	20	
5	555	20	x
6	670	20	x
7	745	20	
8	865	40	x
9	1370	40	x
10	1650	40	x
11	2130	40	x

4.2 Sentinel 4 Level 1B Requirements

The Sentinel 4 is a mission in a geostationary orbit focussed on air quality applications in Europe. The Level 1B requirements for the UV-VIS-NIR (UVN) spectrometer have been studied in CAMELOT.

During the CAMLOT project, the decision to the merge Sentinel 4 and the EUMETSAT MTG programme 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. We refer to http://www.eumetsat.int/groups/pps/documents/document/pdf_mtg_rep38.pdf for a comparative analysis of the MTG-IRS expected performances for chemistry /air quality applications.

4.2.1 UVN spectrometer

The Sentinel 4 UVN spectrometer will be used to measure the concentration of the following tropospheric trace gases: ozone, nitrogen dioxide, sulphur dioxide, formaldehyde and brome oxide. In addition it provides information on aerosols and clouds.

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

The Level 1B requirements for the Sentinel 4 UVN have a large overlap with those for the Sentinel 5 UVN described in Section 4.1.1. Because no vertical information in the stratosphere is required, the Sentinel 5 UVN can spectral range can start at 305 nm instead of 270 nm. Under the assumption that the water vapour product is available from the MTG-IRS, the NIR channel can start at 750 nm, instead of 710 nm. The recommended spectral bands are given in Table 4-8.

Table 4-8. Recommended characteristics for the spectral bands for the Sentinel 4 UVN.

Band	**Spatial Resolution [km]**	**Spectral Range [nm]**	**Spectral Resolution [nm]**	**Sampling Ratio**	**SNR[1,5]**	**Driving species**
UV	≤15 (≤5)	305-380	≤0.5	≥3	550 @ 310 nm (750 @ 320 nm)	O_3 (SO_2, CH_2O)
VIS	≤15 (≤5)	360-500	≤0.5	≥3	1500 @ 420 nm	NO_2
NIR	≤15 (≤5)	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 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.*
5) *The reason for the different SNR values as compared to the Sentinel 5 UVN (Table 4-4) is that a different reference spectrum is defined for Sentinel 5.*

5 Assessment of Cloud Contamination and Optimisation of Mission Scenarios

The impact of cloud was assessed in two ways:

- 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. These statistics were mainly based on one year of SEVIRI data sampled once per hour, generated by the CM-SAF and provided to this project by DWD. Geostationary data was vital as it was the only means of basing simulated GEO and LEO observations starting from the same original cloud dataset.
- In Task 5, statistics on the likelihood of good L2 retrievals (i.e. compliant with user requirements) 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". Statistics on the occurrence of "compliant" retrievals are then accumulated by applying this approach to the full cloud data set. In this way, the cloud field was sampled correctly for each specific orbit type, including the co-variance of retrieval sensitivity to view / solar geometry and surface albedo.

In each case statistics were produced as a function of

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

Some issues could not 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.

Geographical regions have been defined within which the cloud data set was sampled to generate statistics. We primarily consider 240 × 240 km regions centred on London, Madrid, Athens Kampala, Cairo and a location over the Atlantic (up-wind of Europe).

Analysis focused on two statistics:

- P1, the likelihood of obtaining at least one cloud-unaffected observation within a given field-of-regard (FOR), within a given time-window.
- N1: The mean number of individual integration periods that have at least one cloud unaffected observation within the field-of-regard, over the whole time-window, provided at least one time-window has at least one cloud free observation

Both are assessed as a function of

- Location
- Time of year (P1 also assessed as function of time of day)
- 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, in the range 10 to 50 km (square).
- The size of the field-of-regard (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). We analysed FOR in the range 10 – 120 km, with particular emphasis on 20 and 60 km which are commensurate with the threshold requirements on spatial resolution for boundary layer and tropospheric column products, respectively.
- 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 the case of L2 sampling statistics these thresholds are functions of observing / solar geometry and surface albedo.

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.

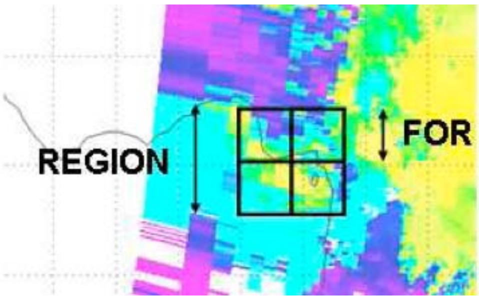

Figure 5-1. Figure shows a swath of polar orbit data. Each coloured tile represents a ground pixel increase in size toward the edge of the swath. The swath passes over a region which, in this case, comprises 4 fields of regard (FOR).

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.

Another important consideration is how the instrument field-of-view (FOV) is assumed to vary away from direct nadir viewing. Two assumptions were considered:

- *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.

Figure 5-2 shows some example results based on geostationary cloud-free sampling for London. This illustrates the expected strong dependence of P1 and N1 on the FOR and pixel size, i.e. the smaller the pixel and the larger the FOR, the better the chance of having one or more good observation in a given time window.

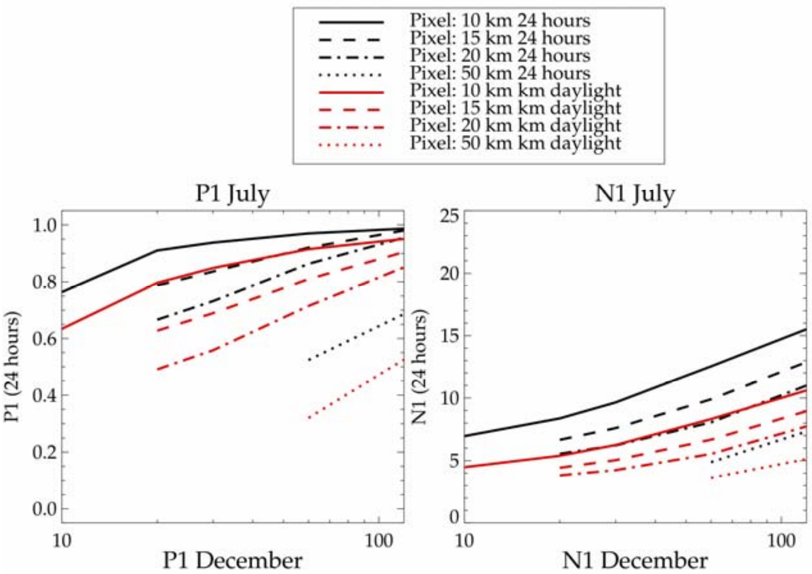

Figure 5-2. Example cloud-free sampling statistics for London in July, comparing various FOR and pixel size. Left-hand panel shows P1 for geostationary orbit over London as a function of FOR size. Right-hand panel shows corresponding values of N1. Red lines show results for obtaining an observations during the sun-lit day; black lines show the statistics for 24-hours. Different line-styles show results for different ground-pixel sizes.

Statistics for a range of orbit scenarios were compared. Figure 5-2 illustrates how observations during a day and for multiple orbit combinations accumulate to provide the 24 hour and daylight values of P1 (in this case London, July, 10 km 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.

Orbits simulated are:

- Geostationary (GEO) (black)
- Sun-synchronous (SS) orbits (solid, coloured lines):
  - Metop's 9:30 descending node crossing time (red)
  - Combination of both 9:30 and 13:30 (orange)
  - Combination of 9:30, 13:30 and 15:30 (brown)
  - Combination of 9:30, 13:30 and 17:30 (light green)
  - Combination of 9:30, 13:30, 15:30 and 17:30 (dark green)
- The combination of 4 non sun-synchronous (NSS) polar orbiters, with inclination 55°, 6 hours out of phase (grey dashed line).

Figure 5-3 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 (in this case) to be 10 km.

Figure 5-4 illustrates how the daytime / 24 hour statistics vary through the year.

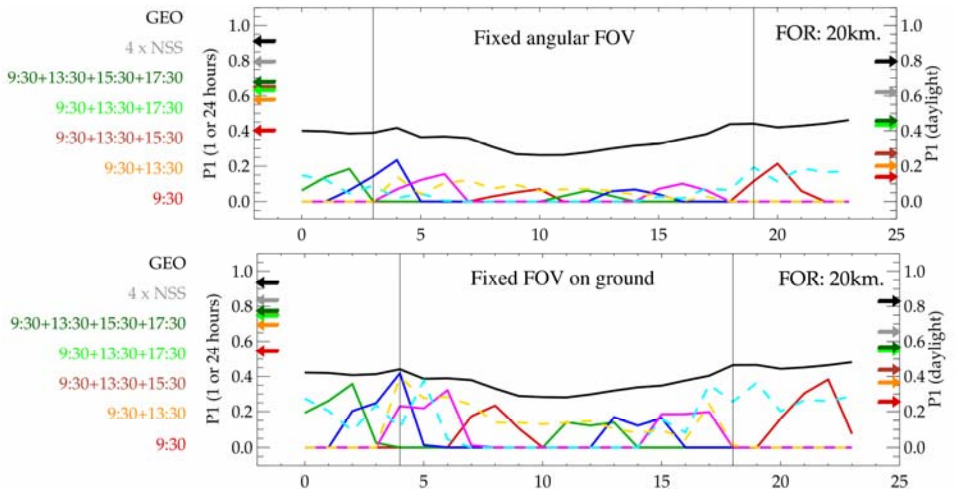

Figure 5-3. Illustration of the accumulation of P1 by combining polar orbits. Results shown are for a 10 km pixel over London in July, considering a 20 km FOR. Lines show the individual hourly sampling from GEO in black and from individual polar orbits in colour. Solid lines show SS orbits and dashed 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).

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 which 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 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. However it was noted that MODIS indicates SEVIRI may under-detect optically thin and / or low-fraction cloud and that therefore “cloud-free” statistics based on SEVIRI may be optimistic if one is interested in observations which are very sensitive to cloud.

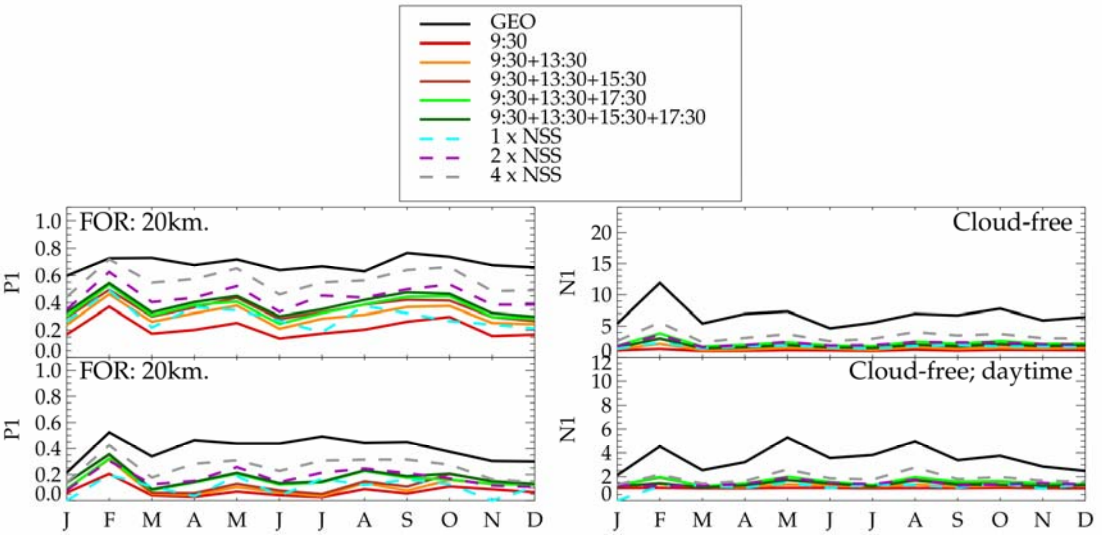

Figure 5-4. Monthly cloud-free sampling statistics for various orbits, for London, for a 20 km pixel size and 20 km FOR. Left-hand panels show the probability of obtaining 1 cloud free pixel over 24 hours (upper sub-panel) or during daylight (lower). Right-hand panels show the mean number of hourly samples found cloud-free, when at least 1 sample is cloud free in 24 hours or during daylight.

Task 5 extended the analysis of cloud-free sampling to compute P1 and N1 for the sampling of Level 2 retrieved products which are able to satisfy user requirements, accounting for retrieval sensitivity to cloud. This mapping between cloud occurrence and other geophysical criteria was accomplished by applying on a pixel-by-pixel basis an operator which determines whether a particular scene is compliant with user requirements.

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. Explicit LUTs were computed for

- 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)

In addition, the cloud-free sampling statistics were considered applicable to height-resolved aerosol from the A-band, CH_4 and CO_2, which are not expected to be usefully retrieved if any level of cloud is present in the scene (or rather, if cloud detectable by SEVIRI is present in the scene). n 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.

An example of the annual mean L2 sampling statistics are illustrated in Figure 5-5.

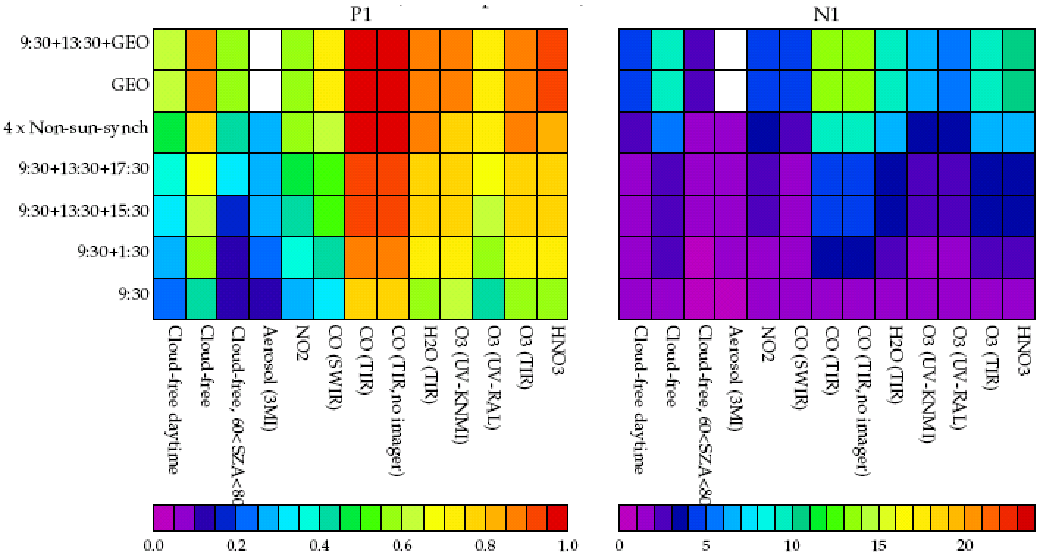

Figure 5-5. L2 Sampling statistics for a 20 km FOR and 10 km pixel size over London. Note that 3MI observations are only relevant for polar orbit (so not shown for GEO). Results for TIR CO with and without the use of an imager to characterise cloud are shown.

Applying L2 sensitivity look-up-tables (LUTs) to simulated scenes, changes statistics 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 60 km (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-ir 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. 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.

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 20 km 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. Still it is the case that 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. However 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 provides particularly 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.

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 0.05 nm 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).

It was noted that 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.

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

6.1 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.

6.2 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 questions 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 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 conclusions 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.
- Applications in the air quality area suggested that it was highly desirable that a satellite product estimating the photolysis rates for NO_2 and easily accessible daily image data of the MODIS form should be produced. The other most desirable aspects were aerosol with dust separation, fires, land cover and land temperature. Sentinels 3 data were recognised to be important for daily image data for all but the first-named data set (photolysis product).
- 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 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 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 10 km 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.

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