TRAQ Performance Analysis and Requirements Consolidation for the Candidate Earth Explorer Mission TRAQ

(TRopospheric composition and Air Quality)

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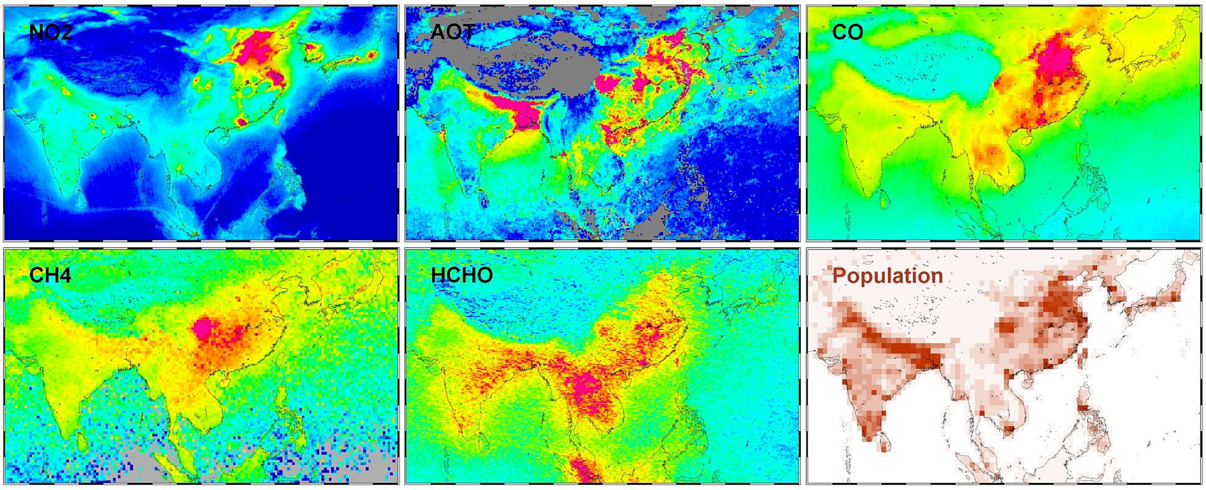

Summary Report

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Figure on front page:

Tropospheric concentrations of key species over Asia, originating from several instruments. Colour scale concentrations range from red, via yellow and green, to blue, which represent very high, high, medium and low values, respectively. For population (lower right) white represent small, and dark brown-red represent large population numbers.

Top left: OMI NO_2. Average over 2007. Note that also the major shipping routes are clearly visible.
Top middle: PARASOL fine mode AOT. Average over the period March 2005 to May 2008.
Top right: MOPITT CO. Average over the period 2000-2007.
Lower left: SCIAMACHY CH_4. Average over the period January 2003 to October 2005.
Lower middle: SCIAMACHY HCHO. Average over the period 2003 to 2007.
Lower right: Population number, in million inhabitants. Acknowledgement: The gridded population density data were obtained from the Center for International Earth Science Information Network (), Columbia University; and Centro Internacional de Agricultura Tropical.

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ESA STUDY CONTRACT REPORT

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ABSTRACT

This report is the executive summary of the ON TRAQ (Original and New TRopospheric composition and Air Quality measurements) study. The key objective of this preface-A study was to support the scientific development of the candidate Earth Explorer Mission TRAQ in parallel to the industrial phase 0 system study for the candidate mission TRAQ.

This project further supported the TRAQ MAG and ESA for the prioritisation of the challenging mission requirements and has provided recommendations to update the Mission Requirement Document (MRD). The output of this study was not fully available for the Mission Assessment Report, written by the TRAQ MAG and ESA. However, initial results of the ON TRAQ project have highlighted the specific science benefits of the TRAQ mission and were used as input for the ESA Earth Explorer User Consultation Meeting (UCM) held in Lisbon on 20-21 January 2009.

This report presents the main conclusions and recommendations of the following three aspects that have addressed in this study:

- Quantitative analysis and consolidation of the mission requirements, as formulated in the TRAQ Mission Requirements Document, including Level 2 and Level 1b data.
- Assessment of the mission performance (Level 2 data).
- Development of an outline architecture and the main features of data analysis algorithms.
- Specific studies in support of the phase 0 industrial studies.
- Specific studies concerning the innovative aspects of this mission (precessing orbit, intelligent pointing for cloud free detection, UV/VIS/SWIR – TIR combined retrievals).

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Introduction

As one of the responses to the ESA's Call for Ideas for the Earth Explorer Core Missions, a mission on **TR**opospheric chemistry and **A**ir **Q**uality (TRAQ) was proposed. The objective of this mission is to contribute to the investigation of tropospheric composition and chemistry, in particular to respond to the following science issues:

- How fast is air quality changing on a global and regional scale?
- What is the strength and distribution of the sources and sinks of trace gases and aerosols influencing air quality?
- What is the role of tropospheric composition in global change?

The proposed payload comprises high resolution spectrometers in the thermal infrared (TIR), shortwave infrared (SWIR), near infrared (NIR) and visible-UV for remote sensing of atmospheric trace gases, as well as a multi-directional polarization imager for detailed aerosol characterisation. These instruments are complemented by an infrared imager for cloud and surface identification. A non sun-synchronous low-Earth orbit is proposed to optimise diurnal coverage at mid latitudes where emissions of air pollutants and climate gases are most prominent.

TRAQ aims to be the first mission fully dedicated to air quality and science issues related to tropospheric composition and global change. The mission aims to deliver high quality, height-resolved information on tropospheric composition with small ground footprints. This is achieved by an optimal synergy of four complementary instruments. The new optimised and non sun-synchronous orbit is proposed to offer near-global coverage and unique diurnal time sampling with up to 5 daytime observations over Europe. With these enhanced capabilities TRAQ will also serve as a cost-efficient comprehensive demonstration mission for future operational monitoring for environment and security.

With TRAQ the following target constituents will be retrieved: O_3, NO_2, CO, CH_4, SO_2, HCHO tropospheric columns; height resolved tropospheric profiles of O_3 and CO and aerosols. Additional parameters include cloud information derived from the infrared imager or from O_2 and O_2-O_2 absorption features in the NIR and visible-UV, as well as surface properties (albedo, effective temperature). Detailed information on clouds, surface albedo and aerosols (and thus light path) will considerably improve the accuracy of TRAQ tropospheric products compared to existing instruments. Moreover, the possibility to make a synergetic use of the instruments on the platform is an innovative aspect of the TRAQ mission, which will allow improving, by suitable combined retrievals, the accuracy and vertical sensitivity of the O_3 and CO distributions in the troposphere. TRAQ aims to fulfil the requirements expected from a tropospheric composition and air quality mission, as those specified in the IGOS/IGACO theme report.

The objective of the present ITT study was to support the scientific development of the candidate Earth Explorer Mission TRAQ in parallel to the industrial phase 0 system study. This ON TRAQ (Original and New TRopospheric composition and Air Quality measurements) project performed the necessary steps for preparing the feasibility phase in case the candidate mission TRAQ would have been selected in February 2009. This project further supported the TRAQ MAG and ESA for the prioritisation of the challenging mission requirements and has provided recommendations to update the Mission Requirement Document (MRD). The output of this study was not fully available for the Mission Assessment Report, written by the TRAQ MAG and ESA. However, initial results of the ON TRAQ project have highlighted the specific science benefits of the TRAQ mission and were used as input for the ESA Earth Explorer User Consultation Meeting (UCM) held in Lisbon on 20-21 January 2009.

The key points of the ON TRAQ study presented in this report include:

- The expected contribution of the TRAQ mission to the understanding of the tropospheric composition in the context of air quality and climate change for a set of representative geophysical scenarios
- The development of geophysical scenarios representative for diurnal variation
- The full traceability matrix from TRAQ mission objectives to level 1 requirements
- Synergistic retrievals for O_3 and CO
- Algorithm concepts, including the development of the on-board cloud detection algorithm
- A study of cloud effects on the sampling strategy of the infrared sounder.

As indicated in the Statement of Work, the following points have been extensively covered:

- Provision of a full set of geophysical (level 2) data requirements for TRAQ using as starting point the preliminary MRD
- Definition of a set of geophysical scenarios to check the mission performance
- Development of a set of Algorithm Concepts and their error analysis, including a dedicated Algorithm Theoretical Basis Document (ATBD) for the cloud imager
- Derivation of consolidated level 1 instrument requirements as described in the Preliminary System Concept of the MRD
- Analyses of the mission performance at the level of geophysical data products for several geophysical scenarios
- Specific sensitivity and retrieval studies to consolidate the level 1 requirements
- Trade-off studies between spatial sampling strategies of the IR sounder
- Analyses of the TRAQ mission contribution in comparison with other existing and planned missions covering several geophysical scenarios typically addressed by the TRAQ mission objectives.

The input for the ON TRAQ project is including the requirements for the TRAQ mission as defined in the MRD. In Task 1 mission objectives have been linked to requirements on the geophysical data products. This resulted in a report with recommendations, which can be used by ESA to update the MRD. In Task 2, about five geophysical scenarios have been considered (and the corresponding model data generated) including scenarios over Europe representative for the diurnal cycle. In Task 3 an overall algorithm architecture and four independent Algorithm Concepts have been developed and tested using existing or *ad hoc* and harmonised codes. The deliverables of this task include the Algorithm Concepts Documents (ACD) together with the corresponding error analyses. One of the geophysical scenarios, i.e. European background polluted, provided by Task 2 and the preliminary algorithms developed in Task 3, have been used as input for sub-task 4.1, in order to consolidate level 1 requirements. Based on the same input but with a larger set of representative scenarios, sensitivity studies have been performed in sub-task 4.2 to evaluate the mission performance. Task 4 results appear in a report providing updated level 1 requirements, comparing mission performances to the actual TRAQ objectives. The corresponding results confirm the chosen algorithm architecture and validate the algorithm concepts. As output of Task 5, the ATBD for the cloud imager on-board processing was a deliverable used by ESA for the technical part of the Mission Assessment Report. An ACD for ground processing of the cloud imager data has been proposed and an overall report includes recommendations for an update of the MRD. In Task 6 simulations were done over Europe using a geophysical scenario covering both low and high pollution situations, based on CHIMERE model fields. Existing satellite data have been used to check the simulation calculations. In Task 7, specific sensitivity studies were performed as needed in Task 1 through 6. Results of Task 7 are reported as part of Task 1-6. All the reports were used as input for Task 8 leading to the overall conclusions of this ON TRAQ project.

1 ON TRAQ Task 1: Review of the TRAQ geophysical data requirements

The main focus of Task 1 of the ON TRAQ project was a review of the geophysical data requirements (level 2 or L2) as given in chapter 4 of the TRAQ Mission Requirements Document (MRD). The TRAQ mission concept includes a novel optimised orbit which offers near-global coverage and unique diurnal time sampling with up to five daytime observations over Europe and other mid-latitude regions. The geographical coverage aspects related to this unique orbit have been studied with the help of multi-annual mean distributions of key pollution components and human population. A review of all TRAQ MRD requirements from a chemical weather point of view was performed, based on a new dedicated analysis of air quality modelling results and air-quality measurements.

Task 1.1 focused on the geographical coverage and temporal sampling requirements. Two dimensional maps and one-dimensional (latitudinal) projections for several key regions are produced for the emissions and concentrations of TRAQ target observables. In collaboration between partners, the following global gridded data sets have been studied: PARASOL aerosol data; OMI nitrogen dioxide; MOPITT CO; SCIAMACHY methane; SCIAMACHY CO; SCIAMACHY formaldehyde; human population; CH_4 emission maps. This work has provided support for the choice of the TRAQ orbit by showing that the main pollution emission and concentration areas and main population areas are well covered by the orbit chosen. A suggestion was made for a small adjustment of the orbit to cover interesting higher latitude regions. Concentration maps were generated in support of the TRAQ Mission Assessment Group activities (used in the Report for Assessment and the presentation during the Lisbon UCM).

The purpose of Task 1.2 was the derivation of the level 2 geophysical data requirements, starting from the three TRAQ science objectives (air quality, sources and sinks, and climate change). Target and threshold values for the horizontal resolution, vertical resolution, temporal sampling, and uncertainties have been addressed. The work is based on the following observational data and model results: hourly surface observations from AirNOW (North America), AirBase (EEA, Europe) and RIVM (Netherlands); high resolution (2.5 km) model simulation from the model MC2-AQ; output of the Canadian AURAMS model: aerosol type and optical depth; output from the French CHIMERE model. These measurements and model results were complemented with information from the literature. As a result an update of the MRD level 2 requirements table has been provided, with several specific recommendations for stronger or weaker requirements. This includes: tropospheric ozone uncertainty and height range (stronger), CO and CH_4 resolution (weaker), NO_2 (weaker), HCHO (weaker) and SO_2 (stronger) uncertainty, SO_2 information for aerosol formation (not in MRD), aerosol layer altitude (weaker) and the air quality index (stronger). An analysis of model results is convenient because of the availability of 3D concentration maps on an hourly basis. However, the models have shortcomings and requirements should ideally be derived from detailed *in situ* measurements. A natural extension of the work was the analysis of campaign data, e.g. aircraft lidar data.

A full account of the work performed in Task 1 can be found in the following report: “ON TRAQ Task 1: Geophysical data requirements”, RP-ONTRAQ-KNMI-024, version 2.1, 20 May 2009).

2 ON TRAQ Task 2: Geophysical Scenarios

The purpose of Task 2 was to provide a chemically and physically consistent set of geophysical input data representative of the time frame 2015 – 2020, as input for the retrieval simulations and other work in subsequent tasks. The work was based on the data base which has been constructed for the CAMELOT project using the ECHAM5-HAM global climate model, the TM5 global transport model and the regional transport model CHIMERE over Europe. In ON TRAQ new ECHAM5-HAM runs have been made with appropriate emissions; control runs for the ECHAM5-HAM output were made as well. This data base was further extended with runs of CHIMERE over Europe, as well as two transects, to provide an appropriate high spatial resolution data base for both gases and aerosols, with geophysical scenarios representative for diurnal variation. The surface albedo data base has been updated and extended. A tool to provide covariances has been delivered as well.

The simulation requirements for the ON TRAQ tasks have been analyzed as discussed in TN-ONTRAQ-FMI-012 Simulation-requirements, issue 3. The required set of scenarios and parameters has been derived from the CAMELOT data base that has been extended in ON TRAQ. Data have been extracted for five locations:

1. European (mid-latitude) background; 46.6°N, 0.8°W
2. European polluted (urban pollution); 52.1°N, 5.2°E
3. China polluted; 31°N, 115°E
4. US East coast polluted; 40°N, 75°W
5. High latitude; 67.0°N, 146.0°E

These scenarios cover most of the needs of the retrieval groups. It is noted that scenario 5 is for an area that is not covered by TRAQ, but it has been included for consistency and was used in the ON TRAQ work of Task 4. Additional scenarios have been generated with the CHIMERE model for two transects, one summer time transect near the coast of Great Britain and one winter time transect in Germany. These transects were used in the TIR retrieval simulations. For the CO simulations by SRON, the temperature profiles and skin temperature from the ECMWF fields on a 1 × 1 grid for 2004 were interpolated to 10 am local time. Furthermore CO and CH_4 fields were adopted from the TM4 model for the year 2004 on this grid. These fields are not averaged in space and time but are provided on the model grid for 10 am.

Model details are summarised in Table 2-1.

Table 2-1. Resolution and data coverage of the models used for the ON TRAQ 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)*	*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*	*2006 / 2008, 4 months*
Availability	*HD sent to KNMI*	*Datasets on ftp*	*Full datasets on ftp*

Tools developed to extract any desired profile from the data base with a resolution of 6 hours for ECHAM and hourly for CHIMERE have been made available. Monthly averaged profiles and their standard deviations for each scenario were computed from the data base made available in digital form.

Other parameters available are the surface skin temperature, high-resolution emission scenarios for CO and the Leicester IG2 carbon dioxide reference atmosphere database.

The applicable period for the TRAQ mission, as specified in the SoW, is 2015 to 2020. The CAMELOT data base includes aerosol, cloud and geophysical parameters for 2015 and trace gases for 2000 and 2030, which is a compromise to include two extremes (for the target year 2015 no emission scenarios are available). The sensitivity to meteorological profiles (temperature and water vapour content) is second order, except for retrievals in the IR part of the electromagnetic spectrum, but inclusion of temperature, water vapour and pressure profiles makes these consistent. There is no need for consistency between trace gas and aerosol scenarios, because the sensitivity of trace gas retrievals for the presence of aerosol can be simulated for a range of aerosol concentrations. CHIMERE provided a consistent data set for both trace gases and aerosols over Europe.

Since the IPCC emission scenarios were developed and used, it appears that the actual emissions changed (especially in Asia). However, it was not possible, given available resources, to update these with more recent information. Rather it has been chosen to use the existing CAMELOT scenarios and analyze these further to provide the extreme situations that may be expected for the TRAQ period 2015-2020 and for the relevant geographical regions, e.g., the polluted regions of Europe, Asia, and the high-latitude regions which may be relevant for climate applications.

Surface albedo compiled from the MODIS, GOME, AVIRIS and ASTER data bases as well as BRDF from Polder (Parasol) were already included in the CAMELOT data base. These data span a wavelength range from the ultraviolet wavelengths (~300 nm) to the thermal infrared (~15 μm). The reflectance data bases 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. In the framework of ONTRAQ, this data base was extended with AVIRIS data.

2.1 Conclusions and recommendations

The data base is described in RP-ONTRAQ-FMI-019. The consortium is confident that this database is representative for the period 2015 – 2020. Five geophysical scenarios were delivered for the data set, i.e. European Polluted, European background for long-range transport, ocean, Asia polluted and high latitude regions for the permafrost study in Task 4. For Europe, data with high temporal and spatial resolution was delivered. The data base has been used in Tasks 3 and 4 to simulate retrievals, and is available for use in other simulations as well. Future work should include updates reflecting changes in emissions, especially in Asia. The surface reflectance database is recommended to be used for the simulation of the variability in the surface reflectance to determine the instrument requirements (Note that in this report we use level 1 or L1; we do not introduce L1b here assuming that L1 means in general “calibrated spectrally and radiometrically”).

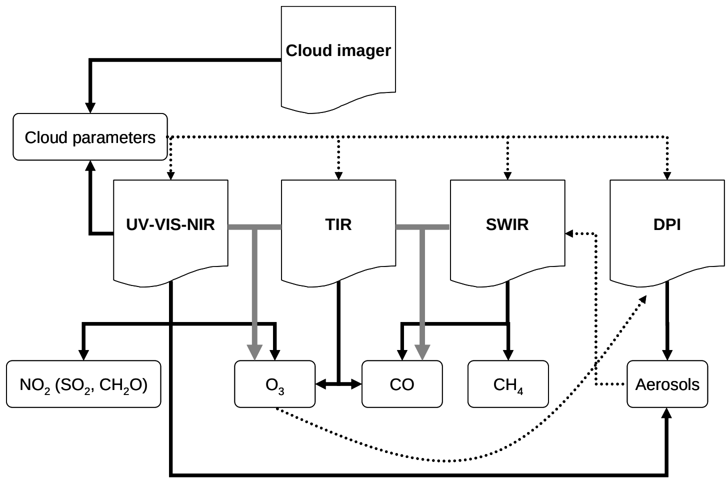
3 ON TRAQ Task 3: TRAQ algorithms

To meet its science goal in tropospheric chemistry and climate, TRAQ targets simultaneously a range of gaseous trace species and aerosols, using complementary observation principles, from imagers to high resolution spectral sounders. Considering the originality of the mission, the objectives of the work were to

- Build an overall algorithm architecture and develop dedicated algorithms, focusing on retrievals aspects including detailed error characterisations.
- Identify the needed input parameters
- Identify the possible synergies among instruments and analyze how they can best be implemented in the architecture
- Provide algorithm simulators for evaluating the mission performances (Task 4)

During ON TRAQ, an algorithm architecture for the TRAQ mission has been proposed. It was designed to provide from the suite of instruments (a SWS* and a LWS*, a DPI and a supporting IR-img) the entire set of geophysical products needed to meet the mission objectives. These products include vertical profiles, partial and/or total columns for several trace gases and aerosol properties. Prioritisation among the trace gases was made (O_3, CO, NO_2 as priority-1 species; CH_4, SO_2, HCHO as priotity-2 species) to simplify the overall architecture with the priority-1 species driving the processing chain, but without compromising the measurement of the priority-2 species.

Considering the differences and complementarities between the instruments with respect to the observables, the following three types of synergies have been defined:



The *mission synergies* (black line in the Figure) consist in the simultaneous and co-located measurement of the products from the three optical sounders and the DPI on an individual basis. They fulfil most of the mission needs and are given the highest priority in the algorithm architecture, with the algorithm concepts being elaborated around them with the objective of low-risk (relying on well-established theoretical methods) and robustness.

The *instrument synergies* (grey lines in the Figure) aim at improving a specific product by taking advantage of the different vertical sensitivities of at least two instruments to a given observable. As they concern O_3 (from SWS and LWS observations) and CO (from SWS and LWS observations), they are an attractive and challenging part of the mission and have been included in the architecture at different level (at radiance –L1/L1, product L2/L2 or at intermediate levels) without a definitive choice on their actual implementation because of their low level of maturity.

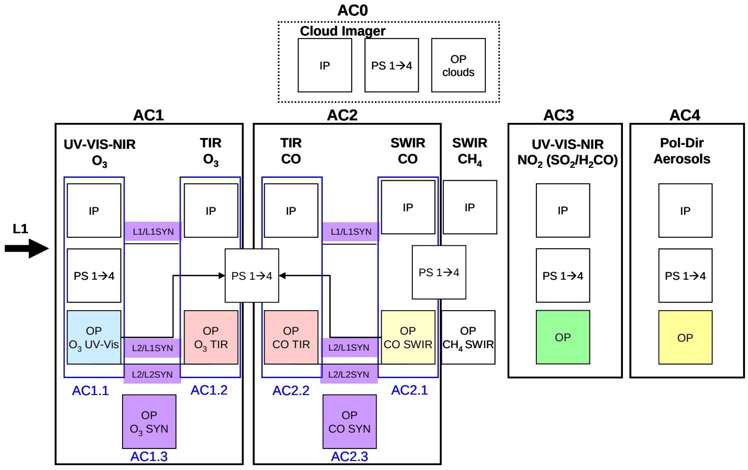
Finally several *indirect synergies*, where the retrieval of a given mission product is subsequently used by another branch of the architecture as an input parameters have been identified.

Relying on the connections between instrument concepts, target geophysical products and possible synergies, the proposed TRAQ algorithm was built on four branches, completed by a supporting branch for the IR-img, as shown in the Figure. They include the following:

- AC0 is the algorithm concept for the on-ground processing of the cloud-imager, which complements the possible on-board algorithm and which aims at supporting the LWS by cloud-clearing/characterising the scene's cloudiness and homogeneity, while also supporting the other optical sounders.

* SWS is the short-wave sounder. It includes measurements in the UV the visible, the near infrared (NIR) and the short-wave infrared (SWIR). LWS is the thermal infrared sounder, with channels in the Thermal infrared (TIR).

- AC1 is the algorithm concept for O_3. It includes three sub-branches: AC1.1 and AC1.2 concern the retrieval of ozone from the SWS and LWS respectively, while AC1.3 provides the synergetic ozone product.
- AC2 is the algorithm concept for CO. It has a similar 3-branches structure with AC2.1 and AC2.2 being instrument-specific (SWS and LWS respectively) and AC2.3 providing the synergetic CO product. AC2.1 can be applied to CH_4 with some adaptations.
- AC3 is the algorithm concept for NO_2, also allowing for the measurements of SO_2 and HCHO. It is linked to the UVN radiance observations.
- AC4 is the algorithm concept for aerosols from the DPI.



Proposed TRAQ algorithm architecture.
IP = Input parameters, **PS** = Processing steps, **OP** = Output parameters.
SYN= Synergies

For each branch a preliminary algorithm concept was developed on a series of processing steps, including geometry and ray-tracing calculations, radiative transfer modelling, retrievals and error characterisation. Their theoretical basis have been thoroughly described and justified and the possible ways of implementing strategies has been reviewed. Furthermore the needs of each algorithm in terms of ancillary data has resulted in a preliminary but already large list of input parameters, being either external or internal (from the indirect synergies) to the mission. These are complemented by a list of local parameters, calculated during the processing but not further kept. The output parameters are documented.

In summary, a first algorithm architecture for TRAQ has been designed to:

- Fulfil the mission needs in terms of geophysical products –profiles or column of trace gases and aerosol properties– and their characterisation (averaging kernels, error covariance matrices etc.). The products were prioritised to alleviate the architecture.
- Benefit from the proposed mission instrument concept, consisting of three optical sounders and a directional-polarization imager, with the support of a cloud imager.
- Maximise the science output by developing synergies wherever possible. Different types of synergies have been identified and their integration in the processing architecture has been proposed based on current knowledge and maturity level:
    - The mission synergies form the core of the algorithm. They allow retrieving from the different instruments on a stand-alone basis a suite of products (at the same location and time) that in itself fulfils the science needs. The level of maturity for the resulting processing chain is high, building on current operational algorithms for e.g. OMI, GOME-2 and IASI. The algorithms have been used to derive L1 requirements and assess the mission performances.
    - The instrument synergies use spectral channels from different instrument to improve on the retrieval of a given product, especially in the lowest layers (troposphere and boundary layer). They concern O_3, from UV and TIR measurements and CO from SWIR and TIR measurements. Such synergies have a high-potential but their implementation is not mature. Possible ways have been described and discussed. The work achieved under Task 4 raised a number of issues; further theoretical investigations are recommended.
    - The indirect synergies consist in using a product from one main processing chain (e.g. cloud parameters from the cloud imager or aerosol properties from the DPI) as input parameter for another chain of the architecture. They are easy to implement and of high importance for the mission. Substantial work has been achieved under Task 4 to quantify the benefit of such synergies. The practical implementation for operational treatment still needs to be made.

Overall, within the algorithm architecture, which has 5 principal branches (AC0 for clouds, AC1 to AC3 for trace gases and AC4 for aerosols), the most innovative aspects concern the implementation of instrument synergies, the development of the on-board processing algorithm for the IR-img, which was conducted as a separate task in the project, and the algorithm development of the DPI. For the others the level of maturity is high and these form the core of the mission. The algorithm architecture is therefore already well-balanced and robust, combining confirmed and innovative algorithmic aspects for tackling the key science questions addressed by TRAQ.

4 ON TRAQ Task 4: Trade-offs, performance analysis and Level 1 requirements

4.1 Introduction

The objectives of the ONTRAQ project Task 4 titled *Trade-offs, performance analysis and Level 1 requirements* was to:

- Derive the level 1 requirements for UV-VIS-NIR, TIR, SWIR and DPI instruments by transferring the requirements in the geophysical parameters into the instrument related parameters.
- Assess the performance of the TRAQ mission using various geographical scenarios, described in Task 2, including studying the advantage of the innovative orbit of TRAQ that allows up to 5 measurements daily and studying the advantage of the unique combination of UV-VIS-NIR, SWIR, TIR and DPI instruments.
- Perform several trade-off studies that were targeted for showing the added value of the TRAQ mission as compared to other missions, for assessing the impact of relaxations of the TRAQ observations and for quantifying specific requirements.

Below, we summarise the results of the Task 4 and, in particular, the synergy between the instruments.

4.2 Instrument level 1 requirements, performance analysis and trade-off studies

4.2.1 UV-VIS-NIR

The UV-VIS-NIR spectrometer is designed to retrieve ozone profiles (UV), tropospheric columns of NO_2 (VIS), SO_2 (UV), HCHO (UV) and information on clouds (UV-VIS-NIR) and aerosol (UV-VIS-NIR) thereby contributing to the science objectives of the TRAQ mission. In addition, the total column of H_2O can be retrieved. Based on simulation studies and the user requirements listed in the MRD new level 1 requirements were derived and compared to the level 1 requirements listed in the MRD. The new requirements are more stringent than those listed in the MRD and more stringent than those obtained from the CAMELOT project. There are two reasons for that. First, the user requirements used in CAMELOT differ from those in the TRAQ MRD, especially the requirements for ozone in the 12 - 18 km and 18 - 24 km sub-columns are more stringent in the TRAQ MRD. Second, the TRAQ MRD specifies that, for ozone, no more than 10 % of the total error budget can have an instrumental origin. This leads to strict requirements in particular for spectral stability and spectral knowledge. In the CAMELOT study it was assumed that 50 % to 100 % of the error budget can have an instrumental origin.

The strict user requirements for the 12 - 18 km and 18 - 24 km sub-columns are not met for ozone. Regarding NO_2, SO_2, and HCHO, the user requirements are not met using current instrument specifications, except for the polluted tropospheric column for NO_2 and strong pollution by SO_2. Requirements on cloud properties derived from the O_2 A-band in the NIR channel are not specified in the MRD. These were derived from a combined retrieval with NO_2, yielding approximately the same requirements as obtained during the CAMELOT study, but the demand that the error due to instrumental effects is less than 10% of the total error budget was ignored here. Simulations performed for spatial stray light show that it should contribute less than 1 % in the UV below 300 nm and less than 2 % above 300 nm, while its contribution in the O_2 A-band should be less than 5 %.

Overall the performance of the retrieval algorithms is as expected. As mentioned earlier, for ozone the requirements are not met for the 12 - 18 km and 18 - 24 km sub-columns. The expected uncertainty there is about a factor of 2 larger than specified in the MRD. For NO_2 the MRD states a maximum allowed uncertainty of 3×10^{14} molecule cm^{-2} on the retrieved tropospheric column. However, the expected uncertainty is 2 - 6 × 10^{14} molecule cm^{-2}. For SO_2 in polluted regions the MRD requirement of 3×10^{16} molecule cm^{-2} can be met, pending some adaptations to the currently proposed instrument characteristics, such as an increase in the SNR from 1000 to 1500. For volcanic SO_2 MRD requirements can be met for total SO_2 columns of 2 DU and larger. For HCHO the threshold in the MRD of 1.4×10^{15} molecule cm^{-2} will not be met, even when the proposed signal-to-noise ratio on the measured radiance would be increased to 2000 (or even 3000).

Simulations for events with increased pollution, based on CHIMERE cases showed that strong pollution events in the lower troposphere with an amplitude of 5-10 DU can be detected with the UV ozone profile retrieval algorithm. The threshold for detection depends on the geometry and the altitude profile of the increased ozone amount. As the error in the retrieved NO_2 column, mostly due to uncertainties in the air mass factor, is of the order of 20 %, daily variations in NO_2 have to be larger than 20 % before they can be detected in a reliable manner. Diurnal variations in SO_2 based on the CHIMERE model results lie far below the detection limit of SO_2 and can therefore not be detected. The same holds for HCHO.

Several specific trade-off studies have been performed.

a) Assuming that one is only interested in the total ozone column, the tropospheric ozone column and tropospheric sub-columns, measurements can start at wavelengths around 300 - 310 nm, depending on the cases considered, such as the geometry and the ozone profile involved.

b) Measurements of the total water vapour column using NIR wavelengths (715 - 720 nm) are accurate to 5 % or better for land and ocean. This is more accurate than the current operational instrument average of 10 % based on TIR measurements, mostly because the NIR observations are sensitive to water vapour in the boundary layer. In particular for measurements over land NIR observations of water vapour have a significant added value.

c) Information on clouds can be obtained using observations in the UV by analyzing the wavelength dependence of the radiance, and by analyzing the effects of Rotational Raman Scattering (RRS). Absorption by O_2-O_2 at visible wavelengths can also yield information on clouds. Finally, the O_2 A-band in NIR can be used to characterise clouds. As the O_2 A-band provides a much stronger signal it can be used to derive additional relevant parameters, such as the surface albedo in the NO_2 fit window. Therefore, measurement of the O_2 A-band does provide substantial additional value and makes it possible to derive cloud parameters and surface albedo values more accurately resulting in more accurate values for O_3, NO_2, SO_2, HCHO and CO.

This leads to the following recommendations:

- Review critically the user requirements listed in the MRD and especially the requirement that no more than 10 % of the final error can be due to instrumental effects
- Adjust the level 1 requirements specified in the MRD so that retrievals for SO_2 meet the user requirements in more cases
- Explore the use of the O_2 A-band further to characterise clouds and surface albedo values as it can lead to substantial improvements in the retrievals, especially for NO_2. Currently only simulation studies have been performed and we are far removed from operational processing.
- Explore user requirements for water vapour. Simulations in NIR above land do give good results compared to current operational products. Should an improved water vapour product be made?

4.2.2 TIR

The TIR sounder targeted for TRAQ mission is optimised to provide vertically resolved information of O_3 and CO in the troposphere, which would contribute to tropospheric chemistry and air quality science objectives of the mission. The instrument design is made considering narrow spectral windows in the thermal infrared: band B1 centred around 1050 cm^{-1} for ozone sounding and band B2 near 2160 cm^{-1} for CO sounding. The study has shown that the sounder specifications were well constrained and provided some possible instrument relaxation, in particular for the spectral resolution in the B1 band. In particular:

With the proposed specifications, the TIR sounder will provide O_3 and CO vertical profiles in the troposphere (2 to 3 independent pieces of information), with a low to medium surface sensitivity, which is mostly driven by the extent of local thermal contrast. The instrument performances for these products can be summarised as follows:

- For O_3:
  - The level 2 requirements are met in most situations, except in the UTLS where the requirement are stringent. Spectral resolution only marginally improves on the performances and a relaxation to an OPD of 6 cm is acceptable. Further relaxation (OPD of 4 cm) should be studied further.
  - The TIR component of the mission would be able to capture, by measuring day and night, some patterns of diurnal ozone variations in case of extreme photochemical pollution in the boundary layer, although with a significant negative bias (underestimation of the pollution level).
  - Large-scale features of the tropospheric ozone profile would be captured by the TIR instrument.

- For CO:
  - The level 2 requirements are tight and met only for low or moderate pollution. High spectral resolution improves on the measurement of CO in the lowest layers and should be targeted (OPD 8 cm) as much as possible, along with low noise.
  - The TIR sounder alone does not allow measuring high CO pollution in the boundary layer with the required level of accuracy due to limited sensitivity near the surface in most cases. There is a strong geophysical limiting factor in reaching this accuracy, which is the temperature gradient close to the surface (temperature contrast). In spite of this, the TIR captures, however, the spatial and temporal variations of CO pollution and is expected to be an essential element of the mission by providing tropospheric measurements day and night above all surfaces

We also recommend looking into the possibility of using the TIR sounder to add information on NH_3 and CH_3OH by a proper selection of channels in B1. This is expected to increase (in particular for NH_3) the TRAQ science output for chemistry and climate applications.

4.2.3 SWIR

The SWIR spectrometer is designed to provide column densities of CO and CH_4. Due to the light path in the SWIR spectral range daytime measurements above land are sensitive to the vertically integrated amount of CO and CH_4 including the contribution from the planetary boundary layer. This makes the SWIR measurements particularly suited to contribute to the science objectives of the TRAQ mission. The study has demonstrated that the proposed one-channel grating spectrometer covering the spectral range 2305 - 2315 nm is well suited to provide the column density of CO and CH_4 with the required accuracy. Here the retrieval of sub-columns is not possible without getting dominated by *a priori* information. It is important to realise that the required SWIR retrieval performance for CO and CH_4 can only be met when measurements of other TRAQ instruments on clouds and aerosol properties are used synergistically. Here spatially and temporally co-located measurements of the SWIR, the UV-VIS-NIR spectrometer in the spectral range of the O_2 A-band and the DPI instrument are essential.

In the ONTRAQ study a set of level 1 requirements on radiometric and spectral properties of the instrument were derived such that the retrieval performance on the CO and CH_4 column density is within the required accuracy. Here general but also specific instrument features (e.g. stray light, memory effect and detector non-linearity) were considered in depth. It is shown that for the purpose of level 1 requirements the variability in the CO and CH_4 abundance is not critical whereas the variations of surface reflectance and solar or viewing geometry have to be considered with care. In this study assumptions had to be made on the overall instrument performance, e.g. the response of the detector device or the hysteresis of the system. The validity of these assumptions depends on the particular design of the instrument and thus it was not possible to verify these assumptions here. Due to that, we strongly recommend to include scientific support during the design and manufacturing of the TRAQ instrument.

To summarise we make the following recommendations:

- Adjust level 1 requirements on the radiometric accuracy of the Earth reflectance measurements in the MRD
- Assure spatial and temporal measurement collocation of the SWIR, UV-VIS-NIR and DPI instrument.

4.2.4 DPI

The DPI radiometer will provide essential and unique information on tropospheric aerosols simultaneously with the trace gas concentrations derived from UV-VIS-NIR, SWIR and TIR instruments. This combination will contribute to reduce the present uncertainties in the processes involved in the aerosol sources, aerosol transport and the transformation of aerosol precursors.

As shown, the present multi-viewing polarization-resolving capabilities of the PARASOL instrument allow a precise characterisation of aerosol load, type and size distribution over ocean using LUT approach for inverting the data. The design of the DPI as well as new inversion scheme will result in similar performances over land. The instrument combines the capabilities of the three sensors that were specifically designed for aerosol studies i.e. MISR, MODIS and POLDER. The instruments are sensitive to different aerosol parameters and the combination of their data will lead to enough constraints for providing all aerosol parameters along one single inversion scheme. The new inversion methodology unifies the principles addressing important aspects of inversion optimisation as accounting for errors in the data used, inverting multi-source data with different levels of accuracy, accounting for a priori and ancillary information, estimating retrieval errors, clarifying potential of employing different mathematical inverse operations (e.g. comparing iterative versus matrix inversion), accelerating iterative convergence, etc (Dubovik, 2004).

As a conclusion:

- With the level 1 requirements listed, aerosol parameters such as the AOD, the size distribution, the percentage of non-spherical particles, the real part of the refractive index, the single scattering albedo (identical in both modes) and the altitude of the top layer can be retrieved.
- If the geometrical conditions (scattering range and number of angles) are not met, AOD and aerosol size can still be derived but parameters related to composition or altitude cannot be obtained.
- The derivation of PM2.5 at the surface level still needs additional studies but the derivation of the altitude of the aerosol top layer, that is a key parameter, should increase the confidence in the correlation between AOD and PM2.5.

4.2.5 IR-img

The two main objectives of the IR imager for ONTRAQ are 1) to provide cloud characterisation and a methodology for the retrieval of cloud parameters in the scene sounded by the TRAQ instruments, particularly to improve the TIR sounding in cloudy conditions, and 2) to increase significantly the number of usable data provided by the TRAQ TIR sounder, by implementing an 'intelligent pointing' strategy, through an on-board algorithm for detection of clouds and/or heterogeneities in order to direct the field of view of the IR sounder IFOV on cloud-free and homogeneous scenes.

The studies on IR-img, presented in Task 3 (on ground algorithm concept), Task 4 (on ground processing in synergy with TIR CO retrieval) and Task 5 (on-board algorithm, performances and interest) reports has shown that the IR-img specifications were well constrained for on-board processing (with some possible level 1 requirement relaxation, e.g., co-registration with TIR sounder, IR-img radiometric resolution and spectral requirements). They do present some strong limitations for the on-ground determination of accurate cloud parameters. However, these limitations should be considered as a second priority if the intelligent pointing is considered as a first priority for the TRAQ mission: in this case observation of cloudy scenes will be minimised, and cloudy/heterogeneous scene retrievals would then be performed in relatively homogeneous or low-contrast conditions.

The on-board processing aspects have been addressed in Task 5. The main conclusion is that the intelligent pointing process is achievable with a simple algorithm concept and should increase the number of useful measurements by a factor 2.7. Considerations on the notion of 'useful measurement' have been briefly discussed, but are still to be examined into more details. An important point is that the optimal pointing shall not only consider cloud-free pixels, but more largely homogeneous measurements. Additional work on these aspects is strongly recommended for TRAQ or similar missions involving TIR sounding in synergy with high resolution IR imagery.

The Task 4 work focused on the processing of cloudy scenes for TIR retrievals in synergy with IR-img information. It has not been possible in the frame of this study to fully address this question. However, some high level conclusions can be drawn: if we limit the objective of cloudy retrieval to some 'relatively simple' scenes, involving in particular cloud fractions lower or equal to 30 % and opaque clouds, with limited complexity in the heterogeneity of the scene (typically only two or three homogeneous components within the LWS heterogeneous pixels), then the necessary parameters (cloud fraction, cloud top temperature/altitude, cloud emissivity, surface temperature, surface emissivity) can be derived from IR-img with the required accuracy, without changes in the MRD specifications. Some limitations occurs in particular for scenes with cirrus or semi-transparent clouds, but would required modification such as 1 or 2 additional channels for the IR-img, and would not represent a large gain for the mission if the intelligent pointing is implemented.

Finally, the MRD baseline of two IR-img basic channels (TIR and MWIR), intended for better detection and characterisation of low clouds, is optimal for on-ground processing and for better correction of the residual cloud coverage (radiance clearing). But this requirement could be relaxed if the intelligent pointing option is selected since in that case the fraction of partially cloudy IFOVs for TIR will be reduced. It is recommended, however, if the MWIR channel of IR-img is not maintained (because of the additional cost/mass/complexity of the cooler), to select two TIR channels for IR-img (in the atmospheric windows on both sides of the 10 µm band of ozone).

This choice is justified by three reasons: it would be a fall-back option for intelligent pointing in case one focal plane array is no longer operation; two TIR channels could be used in real time to still improve intelligent pointing (if margins are available for on-board processing of the imager data); it will provide useful information for cloud characterisation as currently implemented in the split-window technique. A two channel (TIR1 and TIR2) un-cooled micro-bolometer imager of the class of the (single wider TIR band) IASI integrated imager system would meet these requirements.

4.3 Synergy between the instruments

4.3.1 Synergy of UV-VIS & TIR for retrieving ozone

The synergy of the TIR with the UV-VIS is promising in the sense that it will increase the vertical resolution, the sensitivity to the surface and allows for a more accurate measurement of the PBL. This was shown to enhance the capability to track the diurnal variation on qualitative level as compared to the TIR alone. However, more research and software development is needed to address methodological and technical issues that remain.

A combined UV-VIS-TIR retrieval not only gives a better vertical resolution as compared to the individual retrievals and smaller errors, but can also help to control the quality and reliability of the individual retrievals.

A limited effort was made to get a better grip on the system regarding consistency demands. For that purpose inconsistencies were introduced for the absorption cross section in UV-VIS retrievals and significant errors in the retrieved profile were found for inconsistencies > 0.5 %. Presumably, absorption cross sections in UV-VIS and TIR also have to be consistent within 0.5 %. Further, it was found that inconsistencies yield significant differences depending on the type of retrieval (L1-L1 or L1-L2).

This leads to the following recommendation:

- The level of maturity of the combined UV-VIS-TIR has to increase which requires further software development and further research. Our results do show that there is a large potential for improvement in the precision and accuracy of the retrieved ozone profile when UV-VIS and TIR are combined. Further research and, after the level of maturity has increased, tests using measured spectra are recommended..
- Inconsistencies between absorption ozone cross sections in TIR and UV-VIS of 1.0% are expected to give rise to significant bias in the retrieved profile (up to 30% in the troposphere) and / or convergence problems, depending on the retrieval method used. It is recommended to ensure that inconsistencies between TIR and UV absorption cross sections are less than 0.5%.
- As large differences were found for L1-L1 retrievals and L1-L2 retrievals in UV-VIS when inconsistencies were introduced, it is recommended to study all possible combinations of retrievals (L1-L1, L1-L2, and L2-L2) and select the combination that performs best in case of inconsistencies.

4.3.2 Synergy of TIR and SWIR for retrieving CO

The synergistic use of TIR and SWIR stems from the different sensitivities of the channels to the CO vertical structure: The TIR provides vertically resolved profiles in the troposphere with some surface sensitivity (pending on thermal contrast and provided spectral resolution is high), while the SWIR provides uniform sensitivity to the CO column, down to the surface. The study concluded that:

- There is a high benefit for the synergy in case there is a low thermal contrast in the lower troposphere., i.e. when the TIR measurements have limited sensitivity to CO and does not allow for capturing elevated pollution confined in the PBL (see above). The coupling with the SWIR above land allows one to separate CO in the lower troposphere from CO in the free troposphere (vertical resolution is increased), with improved surface sensitivity. The benefit of this retrieval concept was demonstrated for a transect crossing the East coast of the US at 13 March 2000, where temperature and trace gas abundances were adopted from model data. The scenario includes low thermal contrast combined with enhanced CO concentrations in the lower troposphere. Retrieval simulations have shown that in this case the enhanced CO abundance could only be detected properly by a combined SWIR/TIR retrieval. The synergy for CO is of prime interest for addressing the mission science objectives.
- The gain of the synergy as compared to the TIR alone is modest when thermal contrast is high and/or situations unfavourable for SWIR measurements (low albedo).

Critical aspects of the combined SWIR/TIR retrieval have been identified which leads to the following recommendations for a following up study:

- Investigation of the spectroscopic consistency of e.g. trace gas line intensities and widths or absorption cross-sections in both spectral ranges. For CO lines themselves, spectroscopy is not a major issue. What has to be quantified more specifically is the impact of methane spectroscopic errors on the retrieval of the comparatively weak CO lines in the 2.3 μm region.
- Study on the effect of aerosols in the SWIR band, which would be higher than in the corresponding TIR band used for synergistic retrievals. Aerosol information from DPI could be fed into the joint SWIR/TIR retrieval (see Section 4.3.3 below). These issues were not raised in the ONTRAQ study and we thus recommend investigating these aspects in more depth in a follow-up study.

4.3.3 Synergy of UV-VIS-SWIR and DPI

The additional information of aerosols obtained from DPI can be used to improve the UV-VIS and SWIR retrievals. The requirements on the accuracy on CH_4 retrieval are very stringent and require cloud free measurements with only aerosol and cirrus contamination. This means that both cirrus and cloud properties have to be accounted in the retrieval. For this purpose two retrieval approaches are suggested: firstly, a two-band approach is suggested which retrieves effective aerosol and cirrus parameters simultaneously with methane and water vapour from both the O_2 A-band measurements of the UV-VIS-NIR and the 2.3 μm band measurements of the SWIR spectrometer. In the second approach aerosol properties which are retrieved from co-located DPI measurements are adopted in the SWIR retrieval. In this study we showed that

- the required accuracy of the DPI instrument on aerosol optical depth and single scattering albedo is sufficient to retrieve CH_4 within the required accuracy.

Uncertainties on the micro-physical properties of the aerosol and on cirrus cloud parameters were not considered in this study and are recommended to investigate more in future.

In addition, DPI can provide aerosol information that can be useful for the UV-VIS aerosol retrieval:

- the altitude of the aerosol top layer from DPI will result in a more accurate derivation of the aerosol absorption in the UV.

In a reverse way, though the DPI is self consistent, input from other sensors on TRAQ can improve the aerosol retrieval. For instance, the DPI channels that are in the visible part of the spectrum are affected by ozone absorption and thus:

- a simultaneous derivation of the O_3 content from UV-VIS will improve the accuracy of the ozone correction in DPI.

4.4 Discussion

In this project level 1 requirement for UV-VIS-NIR, SWIR, TIR and DPI instruments have been derived based on the geophysical user requirements. Several atmospheric scenarios, including pollution plumes in high temporal and spatial resolution, have been used to assess the performance of the TRAQ mission in various conditions. The user requirements of O_3, CO, CH_4 and aerosol parameters are met in most of the cases but for some of the constituents (HCHO, SO_2, NO_2) the requirements, are so strict that they can not be met or can only be met in some specific conditions. By adjusting the instrument level 1 requirement some improvement can be obtained but it also seems that the user requirements of measuring some of the constituents, e.g. HCHO, background values of SO_2 and NO_2 as well as requirements to measure O_3 and CO in the UTLS region are unrealistic.

General recommendations from Task 4 are:

- The unique combination of UV-VIS-NIR, SWIR, TIR, IR-img and DPI instruments provides to simultaneous measurements of several important constituents needed to study complex processes related to air quality and climate. In addition to that, the combination of instruments can also be utilised for developing novel techniques for improving individual products in the sense of improved vertical resolution, better geographical coverage or higher accuracy. While the benefits of the synergy are demonstrated clearly, more work is needed to fully exploit all the potential existing in the innovative combination of the TRAQ instruments.

- The optimisation of the instrument benefits strongly from simulation studies demonstrating the impact of instrument characterisation at the level of geophysical end products and their error estimates. This scientific support involves testing the instrument characteristics in various realistic geophysical conditions using forward simulations, retrievals, error characterisation and sensitivity analysis. Therefore, it is important to assure scientific support during the design and manufacturing of the TRAQ mission.
- Uncertainties on the micro-physical properties of the aerosol and on cirrus cloud parameters were not considered in this study and therefore it is recommended to investigate the impact of these uncertainties on especially SWIR CH_4 retrieval.

5 ON TRAQ Task 5: Analysis of an intelligent pointing strategy for IR sounding based on on-board processing of the IR imager

This task addresses the assessment of added-value capabilities of the InfraRed (IR) Cloud Imager (or IR-img) for the TRAQ mission: the implementation of an 'Intelligent Pointing' (IP) strategy. The IR imager data can be used through an on-board dedicated detection algorithm to direct the field of view of the IR sounder IFOV on cloud-free or homogeneous scenes. This strategy should increase significantly the number of usable data provided by the TRAQ TIR sounder. However, the scientific merits of this approach have to be estimated with respect to other possible alternatives: simple mono-pixel IR sounder, and IR sounding imager (also called spectro-imager) concept fully mapping the Field of Regard (FOR). The two following points have been addressed:

- specification, development and testing of an on-board 'intelligent pointing' algorithm for the optimised command of the direction of the IR sounder IFOV towards cloud-free or homogeneous scenes
- trade-offs between the scientific merits of the alternative spatial sampling strategies of the IR sounder.

5.1 On board Intelligent Pointing algorithm definition and validation

The baseline for IR-img is a two-channel imager, with TIR (10.8 µm) and MWIR (3.8 µm). From this information, the algorithm definition has been based on several requirements, in particular: select in first priority the position of the sounder pixel for a clear-sky homogeneous IFOV; select in second priority the position of the sounder pixel for a cloudy measurement which maximises the pixel homogeneity; in case of homogeneous cloudy scenes, select in priority low-level clouds. From such requirements, an algorithm has been defined, based on a "minimum" concept:

- using only one channel of IR-img (baseline : TIR channel), an optional (back-up) channel being MWIR.
- combining efficient IFOV selection criteria with system simplicity.

This algorithm concept is thus defined as follows: *Among all potential LWS pointing directions within a given FOR, select the position for which the IR-img minimum signal within the LWS sample is the highest.*

The on-board pointing algorithm has been implemented and applied to MODIS level 1 radiance granules. Compared with central pointing (CP) mode, the intelligent pointing (IP) algorithm is efficient in average, i.e., it favours the observation of hotter and at the same time more homogeneous samples with respect to a central pointing mode. The performance has been assessed in terms of algorithm gain, i.e. the capacity to select the optimum pointing position possible within the FOV. Globally, by using the proposed intelligent pointing algorithm instead of the central pointing mode, 98.0% of the potential brightness temperature increase and 96.5% of the potential brightness temperature standard deviation decrease are achieved. The on-board algorithm thus achieves 97% of the possible gain in terms of radiometry. The intelligent pointing algorithm performance appears stable, at regional scale and at the scale of individual FORs, and does not depend significantly on the LWS spatial resolution.

5.2 Trade-off analysis

In this study we have quantified the number of useful footprints, i.e. footprints which are sufficiently cloud-free, for different observation strategies, such as those possibly employed by the TRAQ IR sounder. High resolution (1 km × 1 km) MODIS TERRA cloud mask observations have been aggregated to lower resolutions. Statistics for different thresholds on cloudiness have been established. For each month in 2004 two days of MODIS data have been analyzed.

We have put a focus on the likelihood of finding a sufficiently cloud-free 10 km × 10 km observation in a Field-of-Regard 50 km × 50 km, employing three methods, in order of efficiency, intelligent mono-pixel pointing (43%-53%), continuous mapping (34%-46%), central mono-pixel pointing (17%-25%).
The intelligent mono-pixel pointing method has the greatest likelihood of finding a single (0%) cloud-free observation (of around 10 km × 10 km) in a 50 km × 50 km region, a factor two and a half when compared to central mono-pixel pointing observations and around a quarter more than for continuous mapping (CM) scanning.

5.3 Discussion

The trade-off study assessed the potential gain of IP mode. Based on the hypothesis that the more useful sample is the less cloudy, a gain factor in terms of useful samples, is estimated to be of 2.1 to 2.7 with respect to the CP mode. In parallel, the validation of a simple and efficient algorithm, implemented and applied on MODIS level 1 data, showed that it is feasible to effectively achieve the potential gain with the proposed on-board algorithm concept.

Because the hypotheses underlying the proposed algorithm, which traduces the geophysical requirements in terms of radiometric criteria, and which considers both the detection of cloud-free and homogeneous scenes, differ from the hypotheses used in the trade-off analysis, open questions remains, and additional work would be required:

- A precise definition of what is a useful LWS sample, with respect to different criteria such as cloud-free scene and homogeneous scene, is to be established. Based on that, the quantification of the homogeneity requirement, as derived from the experience of retrieval accuracy for cloud contaminated spectra, is of first importance.
- Any problems inherent to the MODIS cloud mask are passed to the present investigation (handling of unclassified pixels, or simply MODIS cloud mask errors, etc…). This corresponds, for example, to check for surface heterogeneity, or to consideration of broken clouds without contrast with respect to the surface.
- Additional analysis of the IP performance in selected cases (clear-sky cases with strong surface heterogeneity, individual cases with lowest IP algorithm performance), would be required
- An “improved” concept could be proposed for further study: the TIR and MWIR channels could be processed in real time simultaneously. A selection and/or combination of the optimum IFOV derived from TIR and MWIR would be interesting (depending on the computing power of the on-board IR-img processor).

6 ON TRAQ Task 6: TRAQ Performance Simulation and Comparison to Other Missions

6.1 Introduction

The objective of ONTRAQ Task 6 was to compare the expected TRAQ performance with the performance of current and planned satellite missions. In this task, special attention was given to the TRAQ measurements of the diurnal cycle of the composition of the troposphere, in comparison with existing and future constellations of satellites.

For satellite observations related to air quality, it is essential to have a good spatial coverage, to provide daily measurements of a key set of species including ozone, NO_2, aerosol and CO. The approach to Task 6 was to simulate observations of the current missions, future missions and the TRAQ mission over Europe using a geophysical scenario covering both low and high pollution situations. The simulated satellite observations are derived from the CHIMERE model field. This has been done by simulating overpasses of the various instruments and sampling the CHIMERE data, taking into account the spatial resolution and swath. It is noted that the simulations do not include retrieval simulations, which are covered in Task 4.

6.2 Conclusions

The objective of Task 6 was to demonstrate the performance of the TRAQ mission and compare it to current and future constellations of satellite instruments. To this end simulations have been performed based on CHIMERE model data and a set of tools that have been developed in this task. The tools have been produced or adapted to simulate and visualise satellite observations are:

- Orbsim orbit simulator;
- L2_geo ground pixel position simulator;
- Invgrid interpolates CHIMERE data to ground pixels;
- Gridder produces L3 gridded data from simulated L2;
- Visualisation tools.

These tools simulate the satellite orbits and the satellite measurements by sampling the CHIMERE model data for the ground pixels and spatial coverage of the various instruments. The outputs of these tools are simulated level 2 products, which can be used to produce higher level products, subsets and visualisations. The simulations have been performed for 18 July 2006 00:00:00 UTC until 19 July 2006 00:00:00 UTC, a situation with high ozone concentrations over Europe (See Figure 7-1). The TRAQ simulations have been compared to simulations of Envisat, MetOp and NASA EOS instruments. These simulations have been performed for ozone, carbon monoxide and aerosol optical thickness. The GMES Sentinel atmospheric missions have not been included, because at the time when this work was performed, these missions were not approved.

The visualisations of the simulated data show that the TRAQ data have strong added value, both over the current as well as the future mission constellations. For example the TRAQ NO_2 data provides more spatial and temporal information than the combinations of MetOp/GOME-2 Envisat/SCIAMACHY and AURA/OMI. For the situation after Envisat and AURA the TRAQ data are even more valuable.

Also for carbon monoxide the simulations demonstrate the improved temporal resolution. The combination of SWIR and TIR measurements in TRAQ will enable to distinguish the lower tropospheric layer, in which most of the diurnal variations due to changing emission take place. Thus the combination of temporal and vertical will enable for example the monitoring of the development of wildfires.

The simulation performed in Task 6 demonstrates the added value of the TRAQ non-Sun synchronous observations over current and future satellite missions, for diurnal and vertical sampling. It is noted that the visualisations that have been generated focus on Europe, however he TRAQ mission will provide similar diurnal information for all longitudes at comparable latitudes as Europe, including part of the USA, Canada and East Asia.

7 ON TRAQ Task 8: Conclusions

A key challenge for the next decade is to better quantify the anthropogenic perturbation to the atmospheric component of the Earth system. This is addressed by the TRopospheric Composition and Air Quality (TRAQ) mission. TRAQ will measure key pollutants, radiatively active compounds and their precursors, and will improve the understanding of tropospheric processes. This will provide new insight into how trace gas emissions resulting from human activities are translated into pollution episodes, large-scale tropospheric composition and regional forcings of climate.

The three central scientific objectives of the proposed TRAQ mission are:

(1) Air quality (AQ) and tropospheric composition on a global, regional and urban scale

(2) Trace gas and aerosol emission estimates, chemical transformations and removal

(3) Tropospheric composition changes in their connection with climate.

TRAQ has a unique orbit to capture air quality with near-global coverage combined with the capability to sample diurnal variability over the most polluted regions in North-America, Europe, and Asia. TRAQ aims to combine accurate observation of the chemically active tropospheric constituents with the advantages and cost-efficiency provided by a low-earth orbit. These include a multi-angle viewing geometry which is crucial for aerosol measurements from orbit, and improved accuracy due to higher signal and smaller observation angles over Europe in comparison to a geostationary orbit. In addition, TRAQ remote sensing measurements have sufficiently high horizontal and vertical resolution to probe air pollution in the lower troposphere at urban scales. Furthermore, TRAQ will combine observations of precursor gases with a range of aerosol parameters. The vertical resolution in the troposphere for CO and O_3 is enhanced by the combination of spectral ranges covered by TRAQ: the ultraviolet-visible-near infrared (UV-VIS-NIR), the shortwave infrared (SWIR) and the thermal infrared (TIR).

In order to consolidate the scientific mission objectives of TRAQ, the ON TRAQ consortium lead by KNMI and including experts from European and Canadian institutes was selected by ESA (after an AO on TRAQ studies). The results of the corresponding extensive and intensive investigations by dedicated scientists and engineers have been provided in specific reports and deliverables. Only highlights are provided in this conclusion.

The main results of the ON TRAQ study are:

- An update of the MRD level 2 requirements table based on analyses of model results, with several recommendations for adjustments.
- An extensive geophysical data base was developed with five geophysical scenarios, i.e. European polluted, European background, long-range transport over the ocean, Asia polluted and high latitude regions for the permafrost study. The consortium is confident that this data base is representative for the period 2015 – 2020. For Europe, data with high temporal and spatial resolution was delivered.
- A robust and well balanced algorithm architecture for TRAQ was designed and developed. It combines confirmed and innovative algorithmic aspects for tackling the key science questions addressed by TRAQ.
- An algorithm was developed for the on-board cloud imager.
- Requirements for the level 1 for the UV-VIS-NIR, TIR, SWIR and DPI instruments were derived by transferring the requirements in the geophysical parameters into the instrument related parameters.
- The performance of the TRAQ mission was assessed using selected geographical scenarios demonstrating the advantage of the innovative orbit that allows up to 5 measurements daily and exemplifying the unique combination of the UV-VIS-NIR, SWIR, TIR and DPI instruments.
- Several trade-off studies were performed that were targeted for showing the added value of the TRAQ mission as compared to other missions, for assessing the possible impact of relaxations of the TRAQ observations and for quantifying specific requirements.
- The simulations performed as a synthesis of the various tasks of the ON TRAQ project demonstrate the added value of the TRAQ non-Sun synchronous observations (over current and planned satellite missions) for diurnal and vertical sampling. Visualizations that have been generated focus on Europe (See Figure 7-1), however, the TRAQ mission will provide similar diurnal information for all longitudes at comparable latitudes as Europe, including part of the USA, Canada and East Asia.

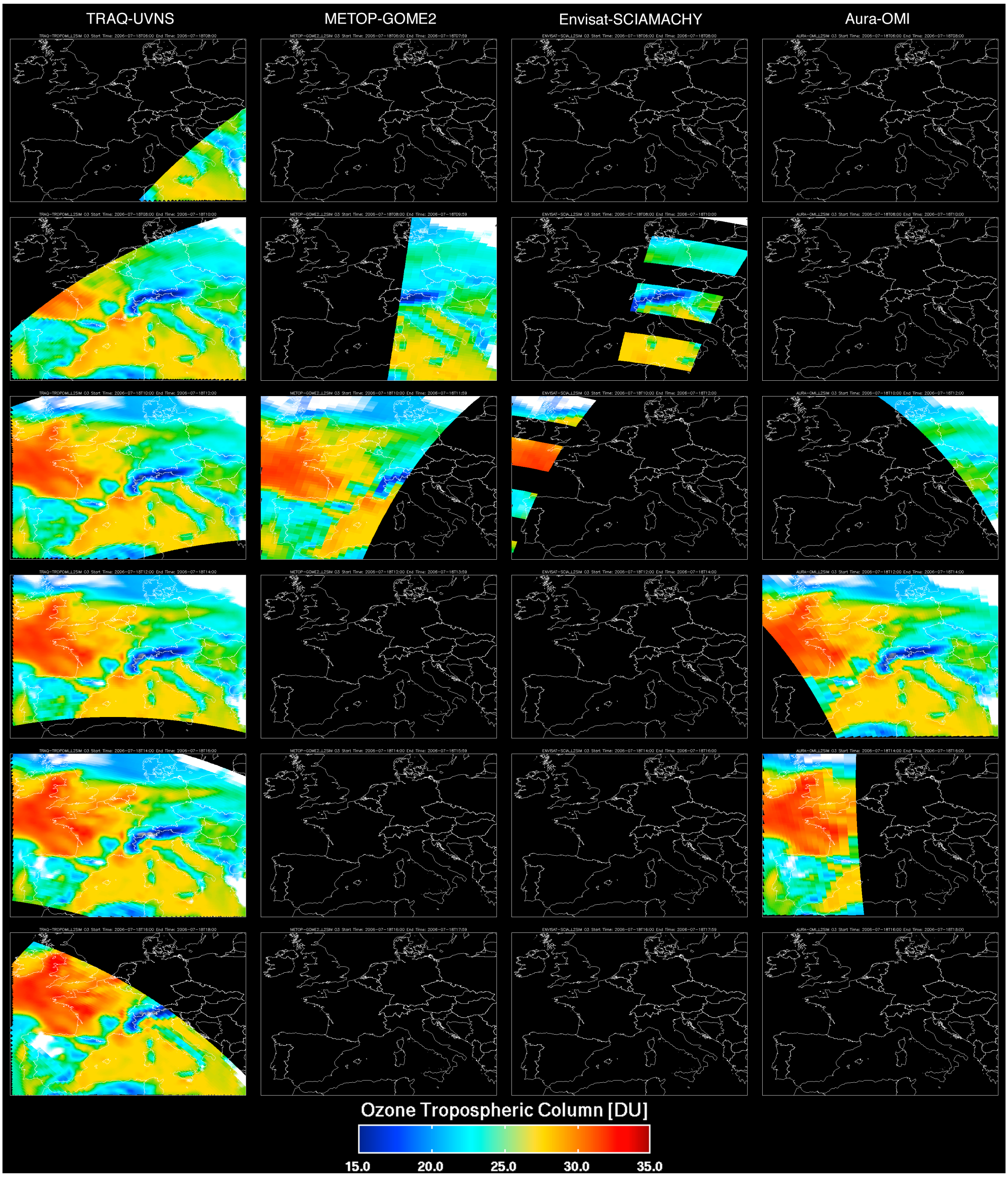


Figure 7-1 *Simulated observations of tropospheric ozone from the UV spectral region. The columns are for UVNS on TRAQ, GOME-2 on MetOp, SCIAMACHY on Envisat and OMI on AURA. The rows are for different time periods with an interval of 2 hours, starting on 18 July 08:00 UTC and ending on 18 July 18:00 UTC. Pixels affected by cloud contamination are coloured white.*

The overall conclusions of the ON TRAQ study are:

- The combined suite of TRAQ instruments enable for the first time the simultaneous measurements (for the same local time and air mass) of key chemical parameters of the troposphere (O_3, CO, CH_4, NO_2, SO_2, HCHO and aerosols).

- In this project level 1 requirement for UV-VIS-NIR, SWIR, TIR and DPI instruments have been derived based on the geophysical user requirements. Several atmospheric scenarios, including pollution plumes in high temporal and spatial resolution, have been used to assess the performance of the TRAQ mission in various conditions. The user requirements of O_3, CO, CH_4 and aerosol parameters are met in most of the cases but for some of the constituents (HCHO, SO_2, NO_2) the requirements, are so strict that they can not be met or can only be met in some specific conditions. By adjusting the instrument level 1 requirement some improvement can be obtained but it also seems that the user requirements of measuring some of the constituents, e.g. HCHO, background values of SO_2 and NO_2 as well as requirements to measure O_3 and CO in the UTLS region are unrealistic.
- Combined retrievals using the UV/VIS/SWIR and TIR to obtain accurate information on O_3 and CO as well as vertical information in the troposphere have been performed using simulated data. Combined retrieval for ozone show great potential, but should be further investigated and proven using real data (OMI/TES, GOME-2/IASI). Combined retrieval for CO is more robust than for the O_3, but remains to be confirmed on real data. The mission is providing further retrieval combinations that can be used to improve the accuracy of the products (e.g. use aerosol information from DPI for improving O_3, CO and CH_4 retrieval).
- A dedicated IR imager for intelligent pointing with a spatial resolution of 1×1 km^2 and on-board processing of the corresponding images in order to minimize the impact of clouds on the TIR retrievals is a key innovative aspect of this mission. It has been shown by simulations based on actual satellite imagery to be a successful concept that will lead to 2.7 times more cloud free observations than without intelligent pointing.
- It is confirmed that the low-Earth, inclined orbit is a highly powerful aspect of this mission and has never been used before in remote sensing of atmospheric composition, yet provides near-global coverage and unique diurnal sampling of relevant air quality parameters. TRAQ innovative observations turn out to provide a unique amount, up to 5, observations per day, which enable the study of the diurnal cycle for trace gases like ozone, CO and NO_2.

The recommendations of the ON TRAQ study are:

- Update the MRD on level 2 requirements for O_3, CO, CH_4, NO_2, HCHO, SO_2, aerosols, AQ index.
- Future work on the data base should include updates reflecting changes in emissions, especially in Asia. The surface reflectance database is recommended to be used for the simulation of the variability in the surface reflectance to determine the instrument requirements.
- As far as the IR imager is concerned, the requirement of two basic channels (TIR and MWIR) given in the initial MRD and intended for better detection and characterisation of low clouds, is optimal for on-ground processing and for better correction of the residual cloud coverage (radiance clearing). But this requirement could be relaxed if the intelligent pointing option is selected since in that case the fraction of partially cloudy IFOVs for TIR will be reduced. A two channel (TIR1 and TIR2) un-cooled micro-bolometer imager of the class of the IASI integrated imager system would fill TRAQ objectives for the characterisation of clouds and surface heterogeneities.
- The unique combination of UV-VIS-NIR, SWIR, TIR, IR-img and DPI instruments is providing simultaneous measurements of several important constituents needed to study complex processes related to air quality and climate. In addition to that, the combination of instruments can also be utilized for developing novel techniques for improving individual products in the sense of better vertical resolution, wider geographical coverage or higher accuracy. While the benefits of the synergy are demonstrated clearly, more work is needed to fully exploit all the potential existing in innovative combinations of the TRAQ instruments.
- The optimisation of instrument specifications benefited strongly from simulation studies demonstrating the impact of instrument characterization at the level of geophysical end products and their error estimates. This scientific support involves testing the instrument characteristics in various realistic geophysical conditions using forward simulations, retrievals, error characterization and sensitivity analyses. Therefore, it is important to assure scientific support during the design and manufacturing of the TRAQ mission.
- Uncertainties on the micro-physical properties of the aerosol and on cirrus cloud parameters were not considered in this study and therefore it is recommended to investigate the impact of these uncertainties, especially for SWIR CH_4 retrievals at the requested precision.

Recommendations concerning the combined retrieval:

- The level of maturity of the combined UV-TIR has to increase, which requires further software development and further research. Our results do show that there is a large potential for improvement in the precision and accuracy of the retrieved ozone profile when UV and TIR are combined. Further research and, after the level of maturity has increased, tests using measured spectra are recommended.
- Inconsistencies between absorption ozone cross sections in TIR and UV of 1.0% are expected to give rise to significant bias in the retrieved profile (up to 30% in the troposphere) and / or convergence problems, depending on the retrieval method used. It is recommended to ensure that inconsistencies between TIR and UV absorption cross sections are less than 0.5%.
- As large differences were found for L1-L1 retrievals and L1-L2 retrievals in UV when inconsistencies were introduced, it is recommended to study all possible combinations of retrievals (L1-L1, L1-L2, and L2-L2) and select the combination that performs best in case of inconsistencies.
- Investigation of the spectroscopic consistency of e.g. trace gas line intensities and widths or absorption cross-sections in both spectral ranges. For CO lines themselves, spectroscopy is not a major issue. What has to be quantified more specifically is the impact of methane spectroscopic errors on the retrieval of the comparatively weak CO lines in the 2.3 µm region.
- Study on the effect of aerosols in the SWIR band, which would be higher than in the corresponding TIR band used for synergistic retrievals. Aerosol information from DPI could be fed into joint SWIR/TIR retrievals. These issues were not examined fully in the ON TRAQ study and we thus recommend an in depth investigation of these aspects in a follow-on study.

In conclusion, this ON TRAQ study showed the great potential of the TRAQ mission for air quality, emission inventories and chemistry-climate related interactions, using:

- synergistic and combined retrievals for obtaining highly resolved horizontal and vertical information in the troposphere.
- an inclined orbit for tropospheric measurements for diurnal sampling.