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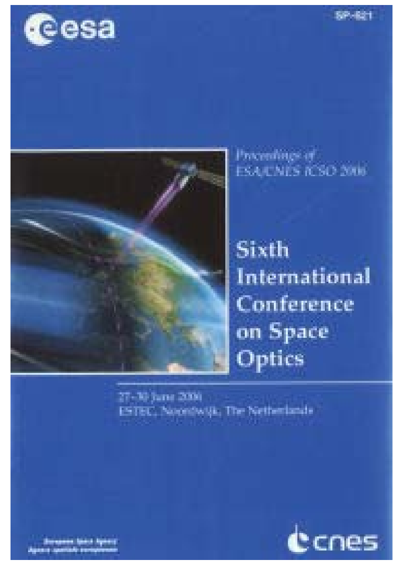

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IMAGING SPECTROMETERS FOR ATMOSPHERE MONITORING

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ABSTRACT

Atmospheric monitoring missions aim at products like O_3, H_2O, NO_2, SO_2, BrO, CH_4, CO, CO_2 as well as aerosols and cloud information. Depending on the application area (Ozone Monitoring, Green House Gas Monitoring, Tropospheric Composition and Air Quality, Chemistry Climate Interaction etc.) total or tropospheric columns as well as profile information is required. The user community of these data as well as their central requirements w.r.t. the payload aspects will be described. A large range of relevant passive instrument types is available, in particular imaging spectrometer, sounder and polarisation measuring systems in the UV-VIS, SWIR and TIR spectral range. Differences between instruments for dedicated missions are highlighted and evolution of requirements is explained, also in comparison with relevant existing instrumentation partly in orbit today. Aspects of technology roadmaps for instrument implementation as well as synergetic effects of instrument combinations and according mission scopes are discussed.

1. Introduction

Space borne spectrometers are a dedicated tool for observation of the atmosphere and to identify and quantify gaseous specimen for scientific monitoring and security purposes. Imaging spectrometers provide us 2 dimensional maps of spectral data, but a second advantage of high spectral resolution is the possibility to retrieve vertical resolution from nadir looking instruments. This is particularly interesting for geostationary instruments which can not offer a limb view like LEO missions, and this at very high repeat cycle in the order of 1 hour and less, comparable with Meteosat. This will set a milestone in global atmospheric monitoring and control, because the high repeat cycle provides a jump in probability of cloudfree observations, which is a general limitation of daily LEO observation especially at northern European latitudes.

Imaging spectrometers hence enable us to monitor motion vectors of atmosphere constituent in a three dimensional manner on a global scale, where full global coverage can only be supported by LEO missions with typically a daily repeat cycle.

This paper gives an overview over instruments which have been studied in the recent years by EADS Astrium GmbH und different ESA and DLR contracts, aiming to implement water vapor motion vectors tracing as well as Air Quality and Atmospheric Chemistry Missions, which are major subjects of the Global Monitoring for Environment and Security (GMES) Program. As such they are considered for Sentinel 4/5, but also to be integrated in other operational missions like MTG and PostEPS or on scientific Earth Explorer Missions.

2. European Atmosphere Programmes

Global Monitoring for Environment and Security (GMES) is a joint EC-ESA initiative, started 1998, aimed at bridging the gap between scientific data produced and useful information needed by governments, environmental agencies and the general public. The overall aim of GMES has been stated in the Final Report for the initial period 2001-2003: *"To support Europe's goal regarding sustainable development and global governance by providing timely and quality data, information and knowledge. - This entails the capacity to have independent and permanent access to reliable and timely information on the status and evolution of the Earth's environment at all scales, from global to regional and local."*. In particular, the GMES information will support Europe in meeting its environmental obligations. It shall contribute to the formulation, implementation and verification of the environmental policies, national regulations and international conventions. Also serving the security of citizens by forecasting and monitoring air pollution and UV radiation events as well as predictions of climate change and its consequences. Priorities selected for the core GMES capacity include support to the EC Environmental Action Programme. Special reference is made to the GMES requirements for Environmental Policy monitoring for Climate Change and Air Quality policy. In parallel to the ESA/EC GMES activities, ESA and EUMETSAT started to define the next generation of their operational

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missions, the geostationary MTG program and the follow on program of the European contribution of the international polar satellite system (post-EPS). The ESA study on future operational atmospheric chemistry missions [1] was an attempt of ESA to summarise the requirements on future missions. In addition, WMO [2] and EUMETSAT [3] prepared position papers on the needs for an integrated atmospheric observing system.

3. Application Areas, User Community and User Requirements

Atmospheric monitoring covers the application areas Stratospheric Ozone and UV, Air Quality, and Climate-Chemistry Interaction [1]. An overview of the application areas is given in Table 1. In each application area user requirements can be traced back to international, European or national protocols, as well as international, European and national needs to forecast and asses the state of the atmosphere on various temporal and spatial scales. The user community is similar wide as the application areas, covering international, European, national and regional acting environmental agencies and institutions. For the application areas three data user categories have been identified: Protocol monitoring, Near-real time data use, Assessment of Trends. Protocol monitoring includes policy support for verification of protocols, legislation and international treaties. Near-real time data use includes both forecasting and monitoring by operational meteorological centres. Assessment includes scientific assessments of long-term environmental threats and associated policy support. The data user requirements are shortly summarized per theme and data user category in Table 1.

For Stratospheric Ozone and Surface UV radiation the protocol monitoring data user requirements stem mainly from the WMO. The future evolution of the ozone layer needs to be monitored over a period of decades. Also, the UV radiation incident at the earth surface needs to be monitored together with information on ozone, aerosols, clouds and surface albedo. Episodes of high UV exposure, dangerous to man, require a forecast system that relies on Near Real Time (NRT) delivery of ozone and some other observations. Vertical resolutions of 2 km or better are required in the upper troposphere and lower stratosphere with temporal coverage of the whole globe in the order of 24 hrs is requested.

Table 1: Application areas and environmental themes, adapted from [1].

Environmental theme // Information need	*Stratospheric Ozone Surface UV*	*Air Quality Local, regional, continental*	*Climate-Atmosphere Composition interaction*
Protocol	UNEP Vienna Convent Montreal and subs Prot. CFC emission verification Strat. ozone halogen distr. trend monitoring	UN/ECE CLRTAP, EMEP/Gothen-burg Prot. EC directives EAP/CAFE AQ emission verification AQ trend monitoring	UNFCCC Rio Convent Kyoto Protocol GHG emission verification GHG/aerosol distribution trend monitoring
Forecast	Stratospheric O3 Surface UV NWP	Local Air Quality (Chemical Weather) Aviation routing Health warnings	Climate scenarios NWP reanalysis
Understanding	Global observations chemistry-transport mod. Stratospheric chemistry UV radiative transport Source attribution WMO assessments UV Health Bio effects	Global, regio, local observation Long-range transport, regio/local BL models tropospheric chemistry source attribution UNEP, EEA assessments Health and safety effects	Long-term global observation System Earth models Transport-chemistry UTLS radiative forcing modelling Source attribution UNEP-WMO IPCC assess Socio-economic effects

Data user requirements for Air Quality protocol monitoring are driven by the EC air pollution directives and the UN ECE Convention on Long Range Trans-boundary Air Pollution (CLRTAP). These include the measurement of aerosol over ocean and land. Further the ground level amounts of aerosol and gases at city are required. For aerosol the demand is for data on particulate matter (PM) at increasingly fine scale, ranging from 10 micron to 2.5 micron. For gases the interest is in ozone and its precursors, nitrogen dioxide, carbon monoxide, and sulphur dioxide. In order to achieve resentative sampling and as a result of the short-term variations of the sources and sinks of these species near the surface, high temporal sampling of 1 hours is needed during daytime. The need to make accurate forecasts of air quality for health and regulatory reasons requires Near Real Time delivery of a similar set of observations, with again a high temporal and spatial sampling frequency day time measurements and night time measurements being desirable.

Climate protocol monitoring requirements are driven by international conventions like the UN Kyoto and concern the emissions of greenhouse gases carbon dioxide, methane, nitrous oxide, and some minority gases. The observational requirements for climate gases arise from the need to improve our knowledge and accuracy of the emission inventories and the sinks for climate gases. This includes both anthropogenic and biogenic sources and sinks. Anticipating potential the future needs, tropospheric ozone and aerosol are also included in these requirements. In this context the precursors of Ozone, such as carbon monoxide and formaldehyde needs to be considered. Climate monitoring and numerical weather prediction by operational centres require Near Real Time availability of several climate relevant gases and aerosols for assimilation. For climate assessment the driver for the requirement is the need to understand climate-chemistry interactions, including radiative, dynamical and chemical processes and feedbacks and their response to global climate change. The requirements include the measurement of water vapour and ozone at 2 km vertical resolution.

4. Data Requirements

Confronting the user requirements with the available data sets from ground based and already firmly planned operational missions like METOP, MSG, NPP/NPOES and GOES, there is a clear need for satellite data addressing the following requirement categories [1]:

(a) High temporal (hourly) and spatial resolution (< 10 km) space-based measurements of tropospheric composition (O_3, CO, NO_2, HCHO, SO_2, PAN, N_2O_5, aerosol) including the planetary boundary layer (PBL) for Air Quality applications. This can be addressed by combined UV-VIS-SWIR (PBL sensitivity) and TIR (tropospheric height information mid troposphere upwards) nadir sounding instrumentation in GEO (driven by high temporal resolution) and LEO (LEO already partly covered by METOP and NPP/NPOESS) covering the relevant spectral ranges of the absorptions and emissions of the targeted parameters. In addition, to properly measure aerosol, multiple angular, multiple polarisation and wavelengths are required.

(b) High vertical resolution measurements in the upper troposphere/lower stratosphere region of O_3, H_2O, ClO/OclO,HNO_3, CH_4, NO_2, BrO, aerosol, etc. for Stratospheric Ozone/Surface UV and Climate applications. A limb sounding instrument suite in LEO using IR, microwave (for sounding under cloudy conditions) as well as UV-VIS instrumentation (O_3, NO_2, BrO) will be able to deliver the required data.

(c) High spatial resolution (< 5 km) and high precision (< 1% for GHGs) monitoring of tropospheric climate and carbon gases (CH_4, CO, CO_2) and aerosols with sensitivity to boundary layer concentrations for climate applications. Here the high precision requirement and the sensitivity to the PBL can be addressed by combined SWIR-IR nadir sounding from LEO. Attention has to be paid to characterise the scattering characteristics of the lower atmosphere by accompanying measurements of aerosol, clouds and surface albedo.

5. Instruments for dedicated missions

5.1 LEO Limb Missions & Instruments

TIR Limb Sounding is already a proven instrument scope implemented as Fourier Transform Sounder and operating on ENVISAT (MIPAS, developed by EADS Astrium GmbH). Limb sounder measure directly the altitude profile and can provide better height resolution compared to indirect methods in nadir view geometry. The mission objectives of the Michelson Interferometer for Passive Atmospheric Sounding are to support climatology and weather forecasting. Trace gas concentration, like e.g. O_3, NO_2, CH_4, C_2H_6, HNO_3 and water vapour are measured in 3 km vertical and 30 km horizontal resolution. In orbit since 2002, MIPAS has provided valuable scientific data.

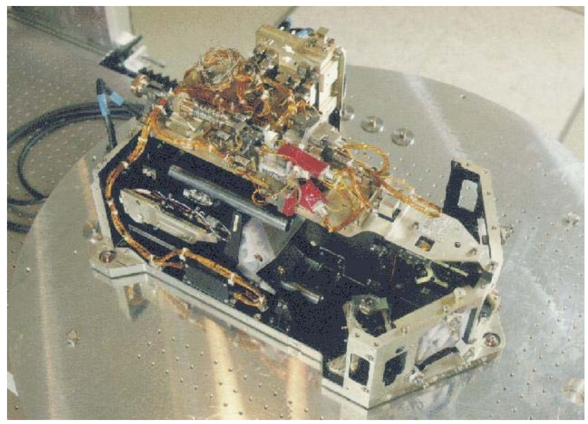

Fig. 1. The core unit of ENVISAT/MIPAS: Interferometer

Next Generation of limb sounders will be equipped like many other new generation high resolution sensors with 2-D detector arrays for enhanced spatial and radiometric resolution. Such a concept has been investigated as an ESA Study on Concepts and Technology for Future Atmospheric Chemistry Sensors in which EADS Astrium GmbH has developed the AMIPAS (Advanced MIPAS) concept and presented preliminary development roadmaps.

Compared to MIPAS on ENVISAT major improvements for the spectrometer are profile measurements with higher vertical resolution without long track shearing at a higher sampling frequency to achieve a dense measurement grid.

Within the next Earth Explorer feasibility studies, the PREMIER mission (proposed by Rutherford Appleton Laboratories, UK) is embarking a limb sounding imaging instrument IMIPAS for which requirements have been defined in cooperation with the Institut für Meteorologie und Klimaforschung (IMK, Germany). The main mission objective is to explore processes controlling the composition of the mid/upper troposphere and lower stratosphere. As a secondary objective, such processes for the lower troposphere/boundary layer and links to other layers are explored. The IMIPAS instrument proposed by EADS Astrium GmbH is similar to AMIPAS, with design modifications in the areas of optics, thermal, detection for improved radiometric resolution, for finer spatial sampling (horizontal & vertical) and for larger field of view

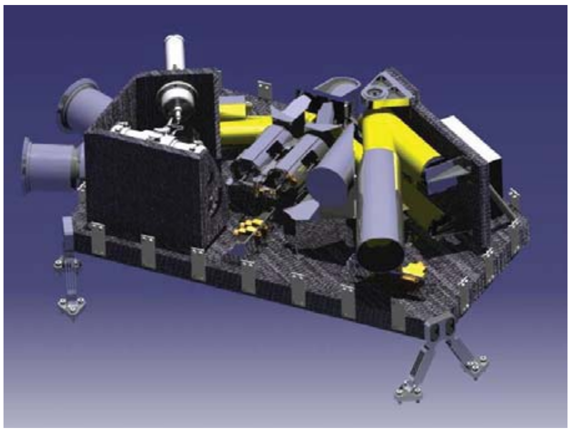

Fig. 2. FTS Limb Sounder "AMIPAS" Phase A Design

UV-VIS Limb Sounding techniques have been established on the European ENVISAT and ODIN missions with the SCIAMACHY and OSIRIS instruments. Both missions demonstrated the robustness of the techniques in a scientific context. Advances in detector technologies would now allow higher spatial and radiometric resolutions and regular spatial coverage with a dedicated instrument. SCIAMACHY and OSIRIS facing their end of operational lifetime, a continuation is therefore to be envisaged.
Planned US missions incorporating a comparable purpose is implemented on NPOESS with the OMPS (Ozone Mapping and Profiler Suite) limb profiler, which objective is however focussed on Ozone.

5.2 LEO Nadir Missions and Instruments

SCIAMACHY is an Astrium GmbH lead high resolution spectrometer on ENVISAT providing ***UV-VIS Nadir Soundings***, while operating in an alternating nadir - limb mode by means of its dedicated scanner unit. A pure nadir UV-VIS scanner is the Global Ozone Monitoring Experiment-2 (GOME 2) which will fly on the MetOp satellites.
A similar US mission is conducted with the OMPS Nadir Mapper included on the operational NPOESS platforms and the Dutch OMI (Ozone Monitoring Instrument) is contributing to the NASA chemistry mission named Aura.

Polarisation Measuring Systems (PMS) especially hunt for anthropogeneous aerosol pollution, which is a serious global problem, because contamination occurs generally at very far distances from its sources as demonstrated in Fig. 3. Here the highest particle concentrations are measured in the coastal areas, which are effected by oversee sources. It is hence a global political issue to trace aerosol sources to detect contaminated areas in order to observe and prevent excessive industrial aerosol expel and to protect the public from constant long term particle strain.
Polarisation measuring instruments are valuable especially to observe aerosol concentration over land. New objective of those instrument are first, that they are dedicated instruments capable to provide several aerosol products like Aerosol Optical Thickness, Refractive Index (both in fine & course mode), Single Scattering Albedo (SSA) and so on, over seas and over land, instead of using available imaging channels, which provide only very limited data, usually only over seas. Principles have been demonstrated by the Polarisation Measuring System (PMS) included in GOME 2. Improvements can be achieved by implementation of additional viewing angles like demonstrated on the French POLDER instrument, which however can not provide regular earth coverage like GOME 2, due to its sequential detection of different channels.

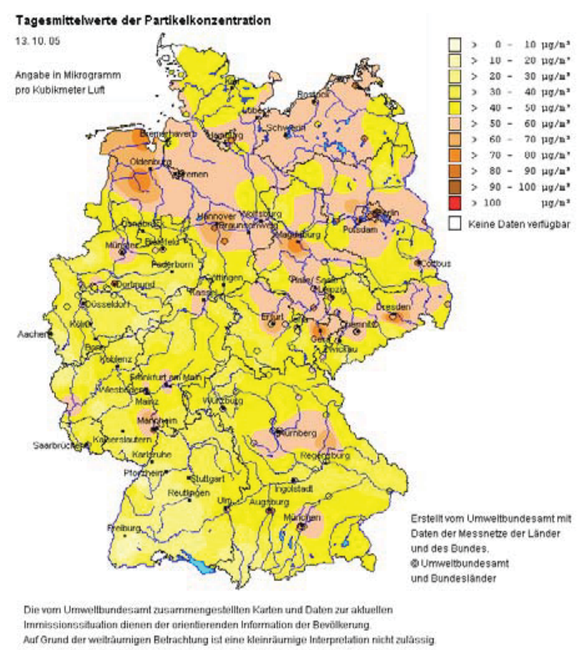

Fig. 3. Aerosol Concentrations over Germany on 13th of October 2005 (Federal Environment Agency)

This class of instrument does not need high spectral resolution, rather in the order of 10 nm but over a large spectral range 350 - 900 nm and needs to observe two orthogonal polarisation states.

Modified dispersive spectrometers or static FTS like the EADS Astrium GmbH FTIS concept have been considered for this field of application.

TIR Nadir Sounding can provide enhanced monitoring of water vapour distribution with good spatial resolution from LEO and to a useful extend also vertical profiles. Current instruments for such missions are IASI on MetOp and the CrIS (Cross-Track Infrared Sounder) on the US meteorological NPOESS platform. Work on IASI successors is only slowly starting, because results from practical experience with this instrument are still awaited.

5.3 GEO Missions and Instruments

There are two main mission objectives which can be served by ***TIR sounding*** from GEO:

- Meteorological, with emphasis on improvement of three-dimensional atmospheric motion vectors by tracing water vapour patterns in support to numerical weather prediction at regional and global scales.
- Chemical weather and Air quality applications, such as vertical profile information on O3, CO, CH4, H2O, N2O and tropospheric column amounts on PAN, C2H6, SO2 (enhanced conditions), HCHO (enhanced conditions) and CFCs.

EADS Astrium GmbH has studied several instrument concepts of GEO Infrared Sounders in the frame of the MTG Pre-Phase A. As an example, a dispersive spectrometer concept is described in the following:

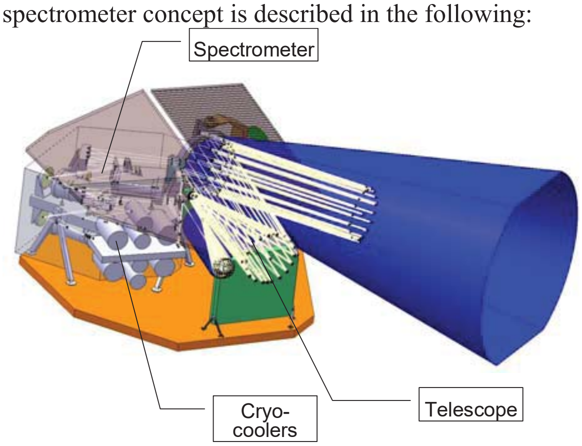

Fig. 4. Optical unit MTG IRS (dispersive option)

The optical unit includes a large sun baffle, a 2 axis scanner, a 300 mm aperture reflective telescope with integrated calibration blackbody, a dispersive spectrometer with collimator, beam splitters, 4 gratings, followed by 4 refractive cameras which focus the spectra onto the various MCT detector arrays. Cryogenic cooling by active pulse tube coolers provides the appropriate temperature level for high performance detector operation at 50 and 80 K, respectively. Passive coolers maintain the spectrometer at an intermediate temperature level and a dedicated thermal design of the front optics evacuates the solar heat load absorbed around midnight. For cloud detection and image navigation, 3 additional cloud imagers are integrated.
The electronic unit is an assembly of several electronic boxes with interconnecting harness. The detector signals are pre-processed in the analogue electronics up to digitisation. Then the digital processing unit provides radiometric corrections and spectral numerical filtering for fine tuning of the instrument spectral line shape function. The data are send to the platform for further compression and downlink. Cooler electronics will drive the cryo-coolers and the instrument control unit assures the instruments command and control as well as the communication with the satellite computer.
The main measurement performances are:

- Spectral range: 4.44 µm-14.3 µm (gap: 6.3…8.3 µm)
- Spectral resolution: 2nm@4.44µm - 25µm@14.3µm
- Spatial sampling at Nadir: 3x3km² / 6x6 km²
- Temporal sampling: Full Earth disc each 30 min
- Radiometric resol.: 0.05K@9µm - 0.4K@5 µm
- 3 integrated cloud imagers at 0.6, 3.8 and 11.4 µm

An instrument serving the MTG Prephase A mission requirements would weight around 300 kg, at > 300 W Power consumption and 180 Mbit/s data rate (before compression).
As a further alternative, a FTS type of imaging spectrometer has been studied as well for the MTG IRS mission, which shows similar interface data but has to deal with higher data rates.
As mentioned before, GEO missions can not provide a limb view, vertical resolutions can therefore only be derived from spectral information, this procedure however requires enhanced high spectral resolution which is easier to increase with FTS concepts. GeoFIS is such an instrument proposed on the GeoTROPE mission, but similar features are assumed on Sentinel 4.

UV-VIS Sounding Missions are driven by the nowcasting objective of atmospheric chemistry and aim at repeat cycles in the order of 30 to 90 minutes and spatial resolution of about 10km over Europe. Required instruments are high spectral resolution

dispersive imaging spectrometer, with 1 or 2 bands in the UV-VIS.
A trend in mission objective has appeared to establish local area coverage, e.g. Atlantic / Europe / Middle East, rather than full disc coverage, but implementing operational flexibility to perform local area coverage anywhere else on the earth disk on request. This leads to longer integration times per pixel and hence relaxes significantly the radiometric instrument sizing.

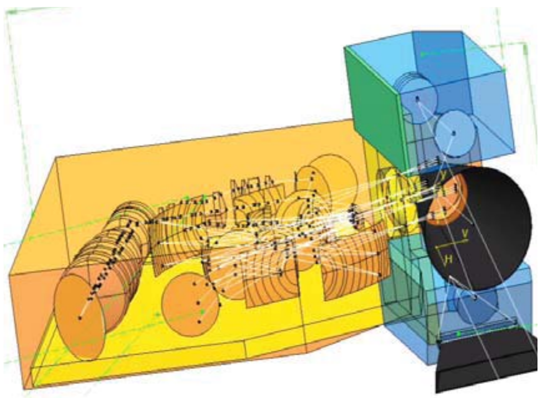

Fig. 5. UV-VIS instrument designed according MTG Pre-Phase A requirements

Within the UV-VIS missions there is the opportunity to equip the instrument with an O2A NIR-spectrometer or a polarisation measuring device for enhanced cloud or aerosol retrieval, while only one of these units is assumed to be included. This leads to compact instrument sizes in the range of 80 to 150kg including electronics depending on the detailed requirements, which makes it a candidate for small geostationary platforms, opportunity missions, as well as complementary payload on MTG or even telecommunication platforms.
The implementation of a SWIR channel however should only be envisaged for very ambitious atmospheric chemistry missions, because for such instruments significantly larger budgets have to be accounted. This is driven by the high requested spectral resolving power (R > 20000) for such a channel, which leads to a large spectrometer size, as well as by the need for powerful detector cooling facilities.

6. Technology Roadmap

Central technical challenge for coming and future imaging spectrometer is the detector technology, because this instrument class requires for all concepts large detector arrays with relatively large pixels imposed by optical constraints and by the required dynamic range. This class of detectors is usually not commercially available, because consumer markets demand compact detectors with high pixel numbers and small pixel sizes. All concepts aim at high radiometric resolution over a large dynamic range which drives the need for fast readout.

6.1 Thermal IR Detectors

Most suitable optical sensitive material is HgCdTe. Predevelopments for HgCdTe-technology have been identified in the frame of MTG and will be launched soon within European detector manufacturers for extension of the cut-off wavelength towards the 14.5 to 15 µm region. The difficulty is to get uniform electro-optical properties and to minimise defective pixels over the large detector areas required. As the dark current is an important contributor to radiometric resolution, this parameter has to be lowered in order to limit cooling down to unusual cryo temperature levels (at a certain stage, further down cooling will not lower the dark current level any more). Read noise and associated dynamic range needs to be improved as well. Large arrays need also to be mastered in view of the thermo-mechanical deformations induced by the mismatch of thermal expansion coefficients between ROIC and MCT materials, when changing from room temperature to cryogenic levels. Further improvements are needed in the area of injection stage. So, detector material, read out circuit and hybridisation of both need major improvements for use in the next generation thermal infrared imaging spectrometers.

6.2. UV-VIS Detectors

Here is a crucial trade to be performed in the area of visible detectors, because high performance scientific grade CCD arrays suffer from significant line transfer times, which simply leads to a loss in integration time for large detector arrays. New CMOS active pixel sensors (APS) provide inherent fast readout capabilities and additionally interesting functionality features, however current poor photon response factors often only in the order of 20% at its peak and difficulties in low noise application, are a strong limitation. According improvement needs are fast readout technologies for CCD's like recently emerged e.g. orthogonal transfer or metal buttressing, which have been demonstrated on laboratory level, but have to be integrated into the mission customized detectors. For the APS technology the main missing brick is backthinning of large scientific grade arrays. For both technologies representative breadboard detector developments are highly recommended, in order to obtain more reliably performance data and reduced risk in terms of development and manufacturing times for space detectors.

6.3 Other technology development needs

Requirements on spectrometer absolute radiometric accuracy as well as on spectral stability have been very demanding for most spectrometer concepts. In this area technology developments seem necessary; however a trade versus relaxation of requirements is necessary if time and cost impact is considered critical.
Related to the high detector transfer rates and data rates the development of according powerful front end electronics (FEE) and digital data processing becomes more and more important.

7. Synergetic Instrument Combinations

For LEO missions IR-Sounder in combination with µ-wave sounder are operating on MetOp and are proposed for PostEPS missions like PEPSIS.
As mentioned, high spectral resolution IR Sounder can provide vertical resolution of products to a significant degree of 3 - 4 layers in the troposphere [4].
An important input parameter for vertical retrievals is the knowledge of the vertical radiance temperature and pressure profile. This can additionally be derived from µ-wave measurement with according bands to observe O_2 and H_2O lines, where these instruments provide more reliable data even from cloudy atmosphere and provide measurement from higher atmosphere layers compared to IR-Sounders.
This applies in a similar way to nadir and limb instrumentation, e.g. STEAM is an according µ-wave limb sounding concept, proposed in combination with IMIPAS on the PREMIER Mission.
A typical IR-Sounder needs additionally high spatial resolution imaging channels, mainly to help detecting cloud covers and fractional cloud cover. Different effective solutions are applicable which have already been investigated for the GEO-IR Sounder.
An alternative is to combine the LEO-IR-Sounder with a more sophisticated high spatial resolution multi-spectral imager in order to address a much broader mission scope like AVHRR with IASI.

For GEO missions combination of UV-VIS Sounding and IR Sounding is proposed on the GeoTROPE mission, which is proposed as a potential candidate for the next Earth Explorer Core Mission. Combination of measurements of back-scattered solar radiance and TIR can provide the best possible passive remote sensing information on the vertical distribution of atmospheric species.
The emission of thermal infrared (TIR) radiation contains information on trace constituents in the troposphere and the stratosphere. TIR radiation is sensitive to tropospheric trace gas concentrations and can be observed both during day and night. This was successfully demonstrated by the nadir viewing ADEOS IMG instrument, and similar data retrieval schemes will be used for the NASA EOS-Aura instrument TES and the EUMETSAT MetOp instrument IASI.

8. Conclusion

A significant number of instrument concepts are available to serve atmospheric monitoring from space in different application areas. Feasibility is demonstrated by several existing missions like on ENVISAT and by many studies conducted on advanced instrument concepts for next generation missions. Promising results w.r.t. to achieving new performance milestones at feasible interface data and costs have been presented.
An overview over the user community of atmospheric data products and application areas has been provided, which is a frequent matter of discussion. Due to the different application areas further prioritisation of the user community themes is a subject. A first approach has been implemented with the 3 topics discussed w.r.t data requirements.

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