Geostationary Satellite Constellation for Observing Global Air Quality: Geophysical Validation Needs

Prepared by the CEOS Atmospheric Composition Constellation

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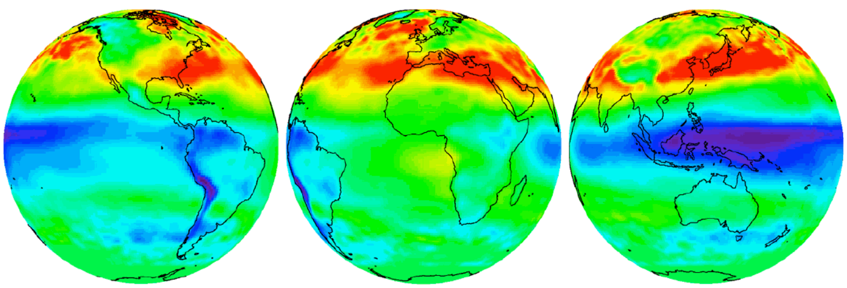

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Cover image: Average tropospheric column ozone in May-July 2008 derived from measurements made bycthe OMI and MLS instruments on the Aura satellite. Purple-blue colors correspond to 10-20 Dobson Unitscand green-red to 35-50 Dobson Units. Image courtesy J. Ziemke, NASA GSFC, and the OMI and MLS instrument and algorithm teams.

List of Acronyms

AAI	Absorbing Aerosol Index
ACC	Atmospheric Composition Constellation
AC-VC	Atmospheric Composition Virtual ConstellationAO Announcement of Opportunity
AOD	Aerosol Optical Depth
AQ	Air Quality
AROMAT	Airborne ROmanian Measurements of Aerosols and Trace gases
C3S	Copernicus Climate Change Service
CAMS	Copernicus Atmosphere Monitoring Service
CDR	Critical Design Review
CEOS	Committee on Earth Observation Satellites
CrIS	Cross-track Infrared Sounder
CLRTAP	Convention on Long-range Transboundary Air Pollution
DOAS	Differential Optical Absorption Spectroscopy
EC	European Commission
EMI	Environment Monitoring Instrument
ESA	European Space Agency
FCI	Flexible Combined Imager
GAW	Global Atmosphere Watch
GEMS	Geostationary Environment Monitoring Spectrometer
GEO-AQ	GEOstationary Air Quality Constellation
GEO-CAPE	GEOstationary Coastal and Air Pollution Events
GMES	Global Monitoring for Environment and Security
GOCI-2	Geostationary Ocean Colour Imager
GOES-R/S	Geostationary Operational Environmental Satellite R/S
GV	Geophysical Validation
IASB-BIRA	Belgian Institute for Space Aeronomy
IASI(-NG)	Infrared Atmospheric Sounder Interferometer (- New Generation)
IRS	InfraRed Sounder
JPSS	Joint Polar Satellite System
KARI	Korea Aerospace Research Institute

LEO	Low Earth Orbit
LI	Lightning Imager
MetOp-SG	MetOp-Second Generation
MTG	Meteosat Third Generation
NASA	National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
NPOESS	National Polar-orbiting Operational Environmental Satellite System
OMPS	Ozone Mapping Profiler Suite
PDR	Preliminary Design review
QA4EO	Quality Assurance framework for Earth Observation
S-NPP	Suomi National Polar-orbiting Partnership
SSA	Single-Scattering Albedo
TEMPO	Tropospheric Emissions: Monitoring of Pollution
TROPOMI	TROPOspheric Monitoring Instrument
TIR	Thermal Infrared
UVN	Ultraviolet + Visible + Near infrared
UVNS	UVN + Short wave infrared
VII	Visible/Infrared Imager (MetImage)
VIIRS	Visible Infrared Imaging Radiometer Suite
WGCV	Working Group on Calibration and Validation
3MI	Multi-viewing, -channel, -polarisation Imager

Reference Documents

RD01 Constellation Concept for Atmospheric Composition, http://www.ceos.org/images/ceosgovdocs/ACC_Concept.pdf

RD02 CEOS, Report of the Committee on Earth Observation Satellites (CEOS) Atmospheric Composition Constellation (ACC) Workshop on Air Quality, http://www.ceos.org/images/ACC-4Reportfinal.pdf

RD03 A Geostationary Satellite Constellation for Observing Global Air Quality: An International Path Forward, Version 4.0, April 12, 2011, http://www.ceos.org/images/ACC/AC_Geo_Position_Paper_v4.pdf

RD04 Requirements for the Geophysical Validation of Sentinel-5P Products, 21 May 2014, S5P-RS-ESA-SY-164 https://earth.esa.int/web/guest/content/-/article/announcement-of-opportunity-sentinel-5-precursor-validation-team

RD05 CEOS Working Group on Calibration and Validation Five-Year Work Plan 2011-2016, Version 5.5, 20 Feb. 2014, http://www.ceos.org/images/WGCV/WGCV_work_plan_v5.5.pdf

RD06 SCIAMACHY Detailed Validation Plan, http://www.sciamachy.org/validation/document/SDVPfinal.pdf

RD07 Ozone Monitoring Instrument Detailed Validation Handbook, TN-OMIE-KNMI-585, Version 1.1, 15. June 2006.

RD08 NPOESS Community Collaborative Calibration/Validation Plan for the NPOESS Preparatory Project OMPS EDRs, No. I30005, VER. 1 REV. B, 5. October 2009.

RD09 Sentinel-5 Precursor Scientific Validation Implementation Plan, EOP-SM/2993/TF-tf, Version 1.0, 1. June 2016.

RD10 A Quality Assurance Framework for Earth Observation: Principles, QA4EO task team, Version 4.0, 14 January 2010. http://qa4eo.org/documentation/

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1. Introduction

The Atmospheric Composition Virtual Constellation (AC-VC) has been initiated by the Committee on Earth Observation Satellites (CEOS) in order to collect and deliver data to improve monitoring, assessment and predictive capabilities for changes in the atmospheric composition. To this end, the CEOS AC-VC strives to coordinate existing and future international space assets and bring about technical/scientific cooperation and collaboration among space agencies. As a space component of the Global Earth Observation System of Systems (GEOSS), the AC-VC addresses directly the GEO Societal Benefit Areas of Disasters, Health, Energy, Climate, Weather and Ecosystems [RD01].

The geostationary atmospheric composition missions Geostationary Environment Monitoring Spectrometer (GEMS, Korea), Sentinel-4 (ESA), and Tropospheric Emissions: Monitoring of Pollution (TEMPO, NASA) have a strong air quality focus and are planned to be launched in the 2018-2026 time frame [RD02]. In the framework of the AC-VC these missions are regarded as the GEOstationary Air Quality (GEO-AQ) constellation. In order to enhance the relevance of the GEO-AQ constellation missions for associated science and policy, AC-VC pursues coordination of algorithm development, harmonization of content and format of the mission products, as well as coordination of calibration and validation activities as laid out in the white paper '*A Geostationary Satellite Constellation for Observing Global Air Quality: An International Path Forward*' [RD03].

At present, this constellation consists of the missions GEMS, Sentinel-4, and TEMPO. In the future, additional geostationary air quality missions might be considered as part of this constellation such as the Geostationary Atmospheric Observation Satellite (Japan) and a FY-4 mission (China). The GEO-AQ missions will be complemented by a number of Low-Earth Orbit (LEO) missions including Sentinel-5 (S5) on the MetOp-SG series, Sentinel-5 Precursor (S5P), Ozone Mapping Profiler Suite (OMPS) on the Suomi-NPP and JPSS satellites, Environment Monitoring Instrument (EMI) on the GaoFen-5 satellite, and potentially other future missions. These LEO mission provide data over regions not covered by the GEO-AQ missions and will provide a travelling standard for assessing and improving mutual consistency between the products of the geostationary missions. A brief overview of the GEO-AQ missions and the above mentioned LEO missions is provided in Section 2. An inventory of current and planned geophysical validation infrastructure is provided in the Annex.

This document aims at identifying

- data products that are common to the GEO-AQ mission (Section 3),
- new validation challenges and inter-mission consistency targets (Section 4),
- needs for coordinated validation activities, new infrastructure and approaches (Section 5).

This document has been written by experts of the geostationary AQ missions GEMS, Sentinel-4 and TEMPO, by members of the CEOS AC-VC, and by members of the CEOS Working Group on Calibration and Validation (WGCV). The objectives of the WGCV are to enhance international coordination and cooperation with a focus on activities in the Cal/Val of Earth Observation for the benefit of the CEOS membership, the GEO and the international user community.

2. GEO-AQ Missions and Related LEO Missions

In this section a brief mission overview is provided for the GEO-AQ constellation elements (GEMS, S4, and TEMPO) and for a selection of related LEO missions (Sentinel-5P, Sentinel-5, OMPS, and EMI).

Although being developed in different programmatic frameworks, the GEO-AQ missions share to a large degree the mission objectives and observational capabilities. TEMPO is a NASA Venture Program mission takes that role of a precursor mission or first element of the atmospheric observational capability of the GEO-CAPE programme. The Sentinel-4 mission is developed by ESA as an element of the Copernicus space component to provide operational measurement for the Copernicus Atmosphere Monitoring Service. The GEMS mission is an operational PROGRAMMATIC FRAME designed to provide operational atmospheric composition data over Asia.

The three missions are implemented as nadir looking grating spectrometers covering the UV, the visible and, depending on the missions, also the near infrared and the short wave infrared. Key mission characteristics are listed for the geostationary (Table 1) and LEO mission (Table 2). The spatial domains covered by the GEO-AQ missions depicted schematically in Figure 1 have essentially no overlap. Amongst the GEO missions, GEMS and TEMPO are expected to be launched first (2018 time frame) followed by Sentine-4 (a few years later). Significant temporal overlap of the three GEO-AQ missions is expected in the years after the S4 launch. The LEO mission OMPS is operational already, while Sentinel-5P and EMI are expected to be flying by the time the first geostationary AQ mission is launched. The temporal overlap of the respective mission lifetimes is shown in Table 3. The GEO-AQ missions and of the LEO missions that complement the GEO-AQ constellation are introduced in the Sections 2.1 to 2.7. The mission products include the key air quality parameters with pronounced temporal variability such as O_3, NO_2, SO_2, HCHO, CHOCHO, and aerosols. Common elements of the product portfolio of the GEO-AQ missions are discussed in detail in Section 3.

Table 1. Key parameters of the GEO-AQ missions GEMS, Sentinel-4, and TEMPO.

	GEMS	Sentinel-4	TEMPO
Orbit	Geostationary	Geostationary	Geostationary
Domain	Asia-Pacific	Europe and surrounding	North America
Revisit	1 hour	1 hour	1 hour
Status	update	Detailed Design Phase, CDR ongoing	update
Host satellite	GEO-KOMPSAT-2B	MTG-S	TBD
Expected Launch	2019	2021 (Flight Acceptance Review first instrument)	No earlier than 11/2018
Payload	UV-Vis 300-500 nm	UV-Vis-NIR 305-500, 750-775 nm	UV-Vis 290-490, 540-740 nm
Products (for details see Tab. 4)	O_3, NO_2, SO_2, HCHO, aerosol	O_3, NO_2, SO_2, HCHO, CHOCHO, aerosol	O_3, NO_2, SO_2, HCHO, CHOCHO, aerosol
Spatial Sampling	3.5 km N/S x 8 km E/W @38N	8 km x 8 km @45N	2.1 km N/S x 4.7 km E/W @35N
Nominal product resolution	7 km N/S x 8 km E/W @38N (gas), 3.5 km N/S x 8 km E/W @38N (aerosol)	8.9 km N/S x 11.7 km E/W @45N	8.4 km N/S x 4.7 km E/W or better @35N (with 100W orbit)
Notes	Synergy with AMI and GOCI-2 instruments w.r.t. aerosol and clouds.	Two instruments in sequence on MTG-S. synergy with IR sounder on MTG-S w.r.t. O_3. Synergy with imager on MTG-I w.r.t. aerosol and clouds.	GEO-CAPE precursor or initial component of GEO-CAPE. Synergy with GOES-R/S ABI w.r.t. aerosol and clouds.

Table 2. Key parameters of the LEO missions Sentinel-5P, Sentinel-5, OMPS and EMI.

	Sentinel-5P	Sentinel-5	OMPS	EMI
Orbit	Low-Earth	Low-Earth	Low-Earth	Low-Earth
Domain	Global	Global	Global	Global
Revisit	1 day	1 day	1 day	1 day
Status	Ready for launch	update	Operational	
Host satellite	Free flyer with only one instrument	MetOp-SG	Suomi-NPP and JPSS series	GaoFen-5
Expected Launch	Summer 2017	2021 (Flight Acceptance Review first instrument)	2011 (Suomi-NPP), 2017 (first JPSS)	
Payload	UV-Vis-NIR-SWIR 270-500, 675-775, 2305-2385 nm	UV-Vis-NIR-SWIR 270-500, 685-773, 1590-1675, 2305-2385 nm	0.3-0.38 µm (nadir mapper), 0.25-0.31 µm (nadir/limb profiler)	
Products (for details	O_3, NO_2, SO_2, HCHO,	O_3, NO_2, SO_2, HCHO,	O_3, NO_2, SO_2, aerosol	

see Table 4)	aerosol, CO, CH_4	aerosol, CO, CH_4		
Spatial Sampling	28x7 km^2 in the UV, 3.5x7 km^2 725-775 nm, 7x7 km^2 elsewhere, @nadir	7 km x 7 km @nadir	50 km (mapper), 250 km (profiler), @nadir	
Nominal product resolution	See above	7 km x 7 km @nadir	50 km (mapper), 250 km (profiler), @nadir	
Notes	In formation with S-NPP for synergy w.r.t. clouds and O_3.	Three instruments in sequence on MetOp-SG. synergy with IR sounder and with imager on same platform.		

Table 3. Expected mission lifetimes of the GEO-AQ missions (red) and the complementing LEO missions (blue).

Year [20**]	15	16	17	18	19	20	21	22	23	24	25	26	27	28	…
GEMS															
Sentinel-4															
TEMPO															
Sentinel-5 Precursor															
Sentinel-5															
OMPS															
EMI															

Figure 1. Schematic view of geographic coverage areas of the geostationary AQ missions.

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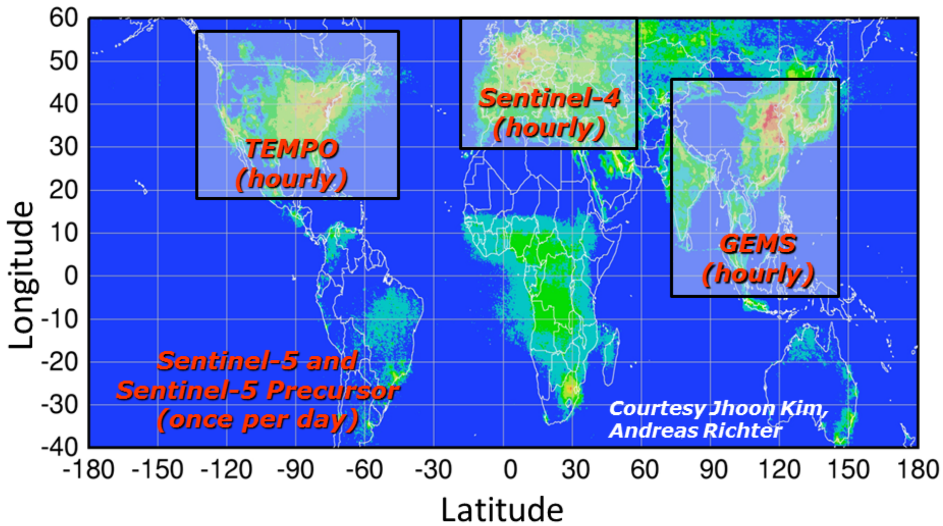

2.1. GEMS

1 page MISSION OVERVIEW, STATUS, APPROACH TO GEOPHYSICAL VALIDATION

2.2. Sentinel-4

The objective of the Copernicus mission ‘Sentinel-4’ is the observation of the tropospheric composition over Europe with a fast revisit time in support of the air quality applications of the Copernicus

Atmosphere Monitoring Services. The Sentinel-4 instrument is an Ultra-violet Visible Near infrared spectrometer (S4/UVN) which is embarked on the geostationary Meteosat Third Generation-Sounder (MTG-S) platforms. Key features of the S4/UVN instrument are the spectral range from 305 nm to 500 nm with a spectral resolution of 0.5 nm, and from 750 nm to 775 nm with a spectral resolution of 0.12 nm, in combination with a low polarization sensitivity and a high radiometric accuracy. The instrument will observe Europe with a revisit time of one hour. The spatial sampling distance varies across the geographic coverage area and takes a value of 8 km at a reference location at 45°N. The key products of the Sentinel-4 mission are NO_2, O_3, HCHO, SO_2, aerosols, and CHOCHO. Additionally, there are dedicated intermediate products for cloud and surface properties. Observations from the Flexible Combined Imager (FCI) on-board the MTG-Imager (MTG-I) platform will be used to enhance the S4 Level-2 product performance. Concurrent observations from S4 and the InfraRed Sounder (IRS) on-board MTG-S will offer enhanced sensitivity to ozone in the lower troposphere, which is to be addressed in future developments.

The development of the S4/UVN instruments and the Level-1b prototype processor is in the detailed design phase and the Critical Design Review is currently ongoing. The Preliminary Design Review of the Level-2 processor development will conclude the algorithm breadbording and the independent verification (spring 2017). The expected launch date of the first MTG-S platform is 2021, and the expected lifetime is 15 years (two S4/UVN instruments in sequence on two MTG-S platforms). The commissioning with a duration of about one year is scheduled after launch. EUMETSAT will operate the S4/UVN instruments and will process the mission data up to Level-2.

It is envisaged that an ESA Announcement of Opportunity for Phase E1 geophysical validation will be issued about 2 years before launch following the S5P approach.

2.3. TEMPO

1 page MISSION OVERVIEW, STATUS, APPROACH TO GEOPHYSICAL VALIDATION

2.4. Sentinel-5 Precursor / TROPOMI

The objective of the Copernicus mission 'Sentinel-5 Precursor' is the observation of the atmospheric composition with daily global coverage in support of climate, air quality, and ozone/UV applications of the Copernicus Atmosphere Monitoring Services. The Sentinel-5 Precursor missions comprises the TROPospheric Monitoring Instrument (TROPOMI) carried on board a dedicated, near polar orbiting platform. The instrument covers the spectral ranges 270-495 nm, 675-775 nm, and 2305-2385 nm with spectral resolutions near 0.5 nm, 0.4 nm, and 0.25 nm, respectively and offers a low polarization sensitivity and a high radiometric accuracy. The along track spatial sampling distance is 7 km at nadir. The nadir across track spatial sampling distance takes values of 28 km in the UV, 3.5 km in the NIR between 725-775 nm, and 7 km at other wavelengths. The mission will be operated in loose formation with NASA's Suomi-NPP spacecraft to allow utilization of cloud information from the VIIRS imager. The key products of the Sentinel-5P mission are NO_2, O_3, HCHO, SO_2, aerosols, CH_4, CO, and spectral UV solar irradiance. Additionally, there is a dedicated intermediate products for cloud properties.

The Sentinel-5 Precursor mission is ready for launch, which is expected for summer 2017. The expected lifetime is 7 years.

In 2014, ESA has released a CalVal Call for the S5P mission. A first issue of the Sentinel-5p Validation Implementation Plan [RD09] has been established based on proposals received in response to this call, will be updated as part of the commissioning preparations.

2.5. Sentinel-5

The objective of the Copernicus mission 'Sentinel-5' is the observation of the atmospheric composition with daily global coverage in support of climate, air quality, and ozone/UV applications of the Copernicus Atmosphere Monitoring Services. The Sentinel-5 instrument is an Ultra-violet Visible Near infrared Short-wave infrared spectrometer (S5/UVNS) which is embarked on the low-Earth orbiting MetOp-SG satellite A. The S5/UVNS instrument covers the ultraviolet (270-370 nm), visible (370-500 nm) near-infrared (685-773 nm), and short-wave infrared (1590-1675 & 2305-2385 nm) spectral bands; the spectral resolution ranges between 0.25 nm for the longest wavelengths and 1.0 nm at the shortest wavelengths. The instrument features a low polarization sensitivity and a high radiometric accuracy. The spatial sampling distance is 7x7 km^2. The key products of the Sentinel-5 mission are O_3, NO_2, SO_2, HCHO, CH_4, CO, aerosols, and spectral UV solar irradiance.

The development of the S5/UVNS instruments and the Level-1b prototype processor is in the detailed design phase and the Preliminary Design Review has been completed at the end of 2015. The Preliminary Concept Review of the Level-2 processor development was completed in spring 2017. The expected launch date of the first MetOp-SG satellite A is 2021, and the expected lifetime is 21 years (three S5/UVNS instruments in sequence on three MetOp-SG A satellites). The commissioning with a duration of about one year is scheduled after launch. EUMETSAT will operate the S4/UVN instruments and will process the mission data up to Level-2.

It is envisaged that an ESA Announcement of Opportunity for Phase E1 geophysical validation will be issued about 2 years before launch following the S5P approach.

2.6. OMPS

1 page MISSION OVERVIEW, STATUS, APPROACH TO GEOPHYSICAL VALIDATION

2.7. EMI

1 page MISSION OVERVIEW, STATUS, APPROACH TO GEOPHYSICAL VALIDATION

3. Constellation Products

In this section, products and parameters that are common to the product portfolio of the GEO-AQ missions GEMS, S4, and TEMPO, are discussed accounting for differences in instrument characteristics and retrieval schemes, which can limit the comparability. Common and comparable elements are referred to as '*Constellation Products*'.

The products of the GEO-AQ missions and the complementing LEO missions are listed in Table 3 (Level-1b) and Table 4 (Level-2). The common elements include the L1b Earth radiance and solar irradiance products and the L2 products for O_3, NO_2, SO_2 HCHO, aerosol and cloud characteristics.

Various approaches need to be followed for the verification of inter-mission consistency. Comparisons of solar irradiance measurements reveal radiometric mismatches, when changes in solar activity, distance to the sun, and Doppler shifts are taken into account. For Earth radiance and Level-2 products one needs to deal with the non-overlapping geographic coverage areas of the GEO-AQ missions. One approach is based on measurements of known targets such as bright clouds or dark ocean scenes. Another approach relies on inter-comparisons with the LEO missions that are used as travelling standard.

The L1b Earth radiance and the solar irradiance products of the three GEO-AQ missions cover a common spectral range from 305 to 490 nm (Table 1). The LEO instruments also cover this range fully (S5P) or partly (up to 380 nm for the OMPS nadir mapper). Level-2 products are derived from reflectance (or sun-normalised radiance), benefitting from a partial cancellation of radiometric calibration errors. Therefore, next to Earth radiance and solar irradiance spectra, also reflectance spectra are considered as Constellation Products, in the common spectral range.

The vertical sensitivity profiles of the L2 ozone profile products differ, depending on the spectral ranges used in the retrieval. The TEMPO mission exploits the ozone absorption signature in the visible (Chappuis band) in order to gain sensitivity to near surface ozone. This feature is not covered by GEMS nor by Sentinel-4. The lower boundaries of the spectral ranges in the UV, limit the stratospheric profile information (especially for Sentinel-4). Accordingly, it is proposed to consider as Constellation Products the ozone total column and various sub-columns covering the stratosphere, the troposphere, the free troposphere, and possibly also the lower tropospheric (0-6 km).

The trace gas total column densities are considered as Constellation Products. Naturally, differences in the retrieval approach (degree of polynomial, treatment of interfering species, fit window, etc) can cause systematic differences in total column data. Therefore, a total column generated using a commonly agreed similar retrieval approach could be added to the products. Such a Constellation Product would facilitate the evaluation of collocated observations by LEO and GEO missions with comparable sun-satellite geometries.

The NO_2 products contain, next total columns, also tropospheric sub-column data. The separation of the total column into stratospheric and tropospheric sub-columns is performed based on several potentially different techniques relying on a-priori data e.g. from chemical transport models. Nevertheless, tropospheric NO_2 sub-columns are considered as Constellation Products in view of their importance for air quality applications.

UV Absorbing Aerosol Index (UVAI) is sensitive to elevated absorbing particles and should take near zero values for cloudy scenes. UVAI data for cloudy scenes can be used to monitor the UV radiometric behaviour. It is expected that the main benefit of such analysis reached already when being applied to the various instruments individually. Does it make sense to consider the UVAI as a Constellation Product?

The comparability of aerosol optical depth data depend critically on the consistency in treatment of surface and cloud characteristics and the assumptions made on aerosol microphysics. IS THERE AN AOD FROM THE LEO MISSIONS? CONSIDER 3MI AS TRAVELLING STANDARD? Does it make sense to consider the AOD as a Constellation Product?

The cloud products are considered as an auxiliary products for the trace gas and aerosol retrievals. Retrieved parameters are effective… …. therefore these products is not geophysically validated.

Table 6. Constellation Products. Common and comparable products and parameters of the GEO-AQ missions.

Product / Parameter	Comparable part	Comment
Level-1b solar irradiance	Spectral subset 305 to 490 nm	
Level-1b Earth radiance	Spectral subset 305 to 490 nm	
Reflectance	Spectral subset 305 to 490 nm	
Ozone profile	Various sub-columns: stratosphere, troposphere, free troposphere, possibly 0-6 km	
Ozone total column	Slant and vertical columns	Additionally, a total column parameter based on a commonly agreed retrieval approach could be considered
NO_2 total column	Slant and vertical columns	
SO_2 total column	Slant and vertical columns	
HCHO total column	Slant and vertical columns	
NO_2 tropospheric column	tropospheric sub-column	Differences in approaches to separation of troposphere and stratosphere play a role

4. Geophysical Validation Targets

Validation is the process of assessing the data quality, in a traceable way. This entails a quantification of the data product uncertainties by independent means, and a verification of compliance of the product performance with the respective requirements. The data quality of independent reference data used for validation purposes needs to be known and documented. Measurements that are regarded as an essential or standard reference for validation of space-borne are referred to as Fiducial Reference Measurements (FRM). A Quality Assurance framework for Earth Observation (QA4EO) has been established in order to ensure that end-users can easily assess whether Earth Observation data are "fit for purpose" [RD10]. Accordingly, products need to contain quality indicators that are based on documented and quantifiable assessments of evidence demonstrating the level of traceability to well defined reference standards. The validation activities for the geostationary AQ missions are needed to provide the basis for the determining the product quality and for the generation of quality indicators. The outcome of the validation process is an essential input to the monitoring of the instruments and the data processors and to the algorithm evolution. A variety of validation activities with different specific purposes needs to be conducted during the mission lifetime (including mission preparation, the mission lifetime and beyond), as outlined below.

Pre-launch

- On-ground characterisation and calibration campaigns are conducted to verify that the instrument flight models are built to design and functional, to characterise the instruments, and to generate calibration key data for data processing. This campaign is typically conducted by the industrial partner building the instrument, and marks a milestone in instrument acceptance by the respective agency. On-ground measurement data from the flight models are of high value for the teams developing the Level-1 and Level-2 processors for functional testing and, e.g. in case of sky measurements, for geophysical testing of the data processors.
- Preparatory validation campaigns ensure that all key elements are ready in time for the activities planned for after launch. This includes the validation strategies, the instrumentation and infrastructure needed for the acquisition of reference data, chemical transport models and other tools needed to interpret reference data and satellite data, and the science community supporting the validation activities.

Commissioning Phase (E1)

The objective of the Commissioning Phase is to verify, after launch, the health of the mission and the correct operating of all its functionalities. After acceptance of the instrument and the Level-1b and Level-2 data processor by the respective agency the satellite is ready for operation.

- Early availability of measurement data (Level-0 and Level-1b) is essential from timely functional testing of the Level-1b and Level-2 processors.
- Light validation activities are conducted during phase E1 aiming at an initial characterisation of Level-1b and Level-2 product uncertainties.

Exploitation Phase (E2)

During the Exploitation Phase, two very different and complementary kinds of validation activities are conducted in order to establish the product quality:

- Validation campaigns are typically geared to collect a variety of reference measurements in selected short periods and limited domains that are collocated with the satellite data. Often, a lot of effort is spent on the acquisition of auxiliary data that characterise the validation scenes in order to support a thorough quantitative understanding of the scenarios. Results of campaigns conducted at the beginning of the Phase E2 are essential input for the consolidation of the algorithms and the initial assessment of the data quality by the Level-1 and Level-2 teams. Follow up validation campaigns are conducted focusing on specific domains, or products. Feedback to the instrument operators is crucial for detection and mitigation of possible anomalies.

- Long-term validation activities are essential for systematic Quality Control of L1B and L2 products, and the operational monitoring of instrument and data processors. For this purpose operational collection of Fiducial Reference Measurements (FRMs) and (to a large degree) automated data handling is needed. A validation database should be employed that allows automated generation of graphs and reports, responding to user queries. Results of such long-term validation activities are essential input for the maintenance and evolution of the algorithms by the Level-1 and Level-2 teams. Feedback to the instrument operators is crucial for detection and mitigation of possible anomalies and degradation of the instrument.

Post Operations Phase (F)

After end of life (Phase F), the mission data are stored, maintained, and kept accessible to users. Re-processing at the beginning of Phase F is usually performed in order to obtain a consistent set of mission data with the best knowledge of calibration key data applied. Additional re-processing campaigns can be necessary to enhance the consistency of the mission data with other long-term data sets. It is vital that metadata and correlative data needed for assessing the mission data quality are stored and kept accessibility to users. Specific validation needs arise from

- re-processing (delta validation of expected algorithm and data improvements),
- development and generation of new data products,
- evolution of data user requirements.

4.1. New Challenges

The validation approach for the geostationary AQ missions builds on the experience from the low-Earth missions (including GOME, SCIAMACHY, GOME-2, OMI, S5P and OMPS) and on the numerous dedicated validation activities that have been conducted in the past and that are currently ongoing or planned (as described e.g. in the validation plans [RD06, -07, -08, -09]).

The GV approach for the geostationary AQ missions needs to address a number of challenges that are specific to the geostationary orbit or new with respect to heritage missions:

a) The capability of sampling the diurnal cycle of atmospheric constituents is a key features of the geostationary AQ missions and is new with respect to heritage LEO missions. This new capability needs to be validated. In particular for short lived species, the GV depends on an adequate treatment of fast chemical reactions, on temporal coincidence of reference data, and on adequate location of these reference data with respect to the sources;
b) The horizontal resolution has been improved as compared to heritage missions in order to reveal finer spatial structure in the atmospheric composition. This enhanced capability needs to be validated, especially for observations near pollution sources, where strong spatial gradients occur. GV of such observations depends critically on the approach to handling mismatches of spatial representativeness between satellite and GV reference measurements, in the vertical as well as horizontal dimensions. At such high resolution the effects of clouds and of orography (shadow) in neighbouring pixels need also to be taken into account;

c) The geographic coverage areas of the different geostationary AQ missions do not overlap spatially. Dedicated approaches need to be found in order to achieve and monitor mutual consistency of the products among the missions;

d) Solar illumination and viewing geometries of geostationary observations vary strongly during the course of a day. Diurnal cycle observations are therefore particularly sensitive to directional characteristics of clouds, aerosols, surface reflectance and orography. GV of diurnal cycle observations depend critically on an accurate description of RT. Availability of appropriate directional information on cloud properties, aerosols, surface reflectance and orography is particularly important for the GV;

e) Obtaining geo-location knowledge is challenging for geostationary sensors, especially in view of the high spatial resolution of the geostationary AQ missions. The geo-location performance needs to be validated; Conversely, GV of geostationary AQ products (see item b) depends on accurate geo-location knowledge.

f) Nadir satellite observations provide little information on vertical distribution; nevertheless the retrieval sensitivity to several species varies vertically. Therefore the quality of vertical distribution information is particularly important for the GV of AQ missions in general.

4.2. Inter-mission Consistency

The impact of the GEO-AQ constellation, and also of each mission individually, is enhanced if the data products are consistent and if this consistency can be demonstrated to the users. One of the goals of future validation activities should therefore be dedicated to the traceable assessment and possibly enhancement of this consistency.

The verification of product consistency is a challenge that requires a combination of various strategies and efforts over extended periods of time. Therefore, it is proposed to establish long-term consistency targets for the systematic differences in Level-1b and Level-2 products between the GEO-AQ missions.

In order to be realistic and verifiable, consistency targets need to be agreed by the science teams accounting for the product performance targets of the individual missions, experience on the consistency of heritage LEO missions, and the accuracy of the verification strategy. Table 6 lists initial values that are discussed and supported in the following sub-sections.

Table 6. Products and systematic differences Goal/Breakthrough/Threshold

Level-2 Product / Parameter	Maximum allowed Systematic differences	Comment
Total ozone column	1-3%	
Tropospheric ozone column	15-25%	
NO_2 total column		
NO_2 tropospheric column		
SO_2 total column		
HCHO total column		

AOD total column		
Level-1b Earth radiance	2-5%	
Level-1b solar irradiance	1-2%	
Reflectance	2-5%	

4.2.1. Ozone

The target performances of Level-2 total ozone product of the GEO-AQ missions are on the order of 3%, out of which only a part will be systematic. Comparisons of various multi-year data records of total column ozone data (SBUV, GOME-type total ozone) and ground-based reference data show that monthly zonal mean values agree at the sub-percent level [*Lerot et al.*, 2014, Chiou *et al.*, 2013]. Long-term consistency of multi-sensor total ozone data records with ground-based reference data on the percent level has been reported [*Koukouli et al.*, 2015]. Ozone trend analyses have been applied to the SBUV, TOMS, and SBUV/2 observations resulting in a data record with trend uncertainty of 1% per decade [Hilsenrath et al., 1997]. A challenging consistency target of 1 to a few % is proposed.

The target performances of Level-2 ozone profile products of the GEO-AQ missions vary substantially, reflecting also differences in the available information content. The S4 target performance for the tropospheric sub-column is 25%. The TEMPO ozone product is expected to provide 0-2 km sub-column data and free tropospheric with 10% precision. What is expected for GEMS? A consistency target better than 15% seems not realistic, in view of the S4 expected performance.

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4.2.2. Nitrogen Dioxide

4.2.3. Sulfur Dioxide

4.2.4. Formaldehyde

4.2.5. Aerosol

4.2.6. Level-1b Earth radiance, solar irradiance and Reflectance

The absolute radiometric accuracy requirements of the GEO-AQ missions constrain the systematic error components to a few percent (2% goal / 3% threshold for S4; NUMBERS FOR TEMPO/GEMS?) for L1b Earth radiance products. Past inter-calibration analyses as performed in the context of the Global Space-Based Inter-Calibration System (GSICS) initiative indicated radiometric consistency of radiances on the 2-5% level [Lacherade et al., 2013]. Absolute radiometric biases of 2% were reported for the visible radiances from VIIRS and MODIS [Uprety et al., 2015]. Consistency targets for Earth radiance are proposed to be set between the consistency of past missions and the expected radiometric accuracy of the instrument.

Inter-calibration analyses yielded calibration coefficients with an accuracy on the percent level [Doelling et al., 2013] accounting for absolute radiometric error contributions such as global offsets and long-term trends for which relative information can be gained in–flight. This level of accuracy might be targeted also for the GEO-AQ inter-mission calibration coefficients.

The absolute radiometric accuracy requirements of the GEO-AQ missions constrain the systematic error components to a few percent (2% goal / 3% threshold for S4; NUMBERS FOR TEMPO/GEMS?) for L1b solar irradiance products. WHAT HAS BEEN REPORTED FOR HERITAGE? Consistency targets for Earth radiance are proposed to be set between the consistency of past missions and the expected radiometric accuracy of the instrument. One might expect same level of consistency as for radiance from a pure instrumental point of view and higher accuracy of inter-calibration knowledge by virtue of stability of the source..

A part of radiometric errors in solar irradiance and earth radiance spectra are expected to cancel out when computing reflectance. The main benefit of this might be in the reduction of spectral features rather than an improvement of absolute radiometric accuracy. Therefore, consistency targets for reflectance should probably be on the same level as for radiance.

References:

Sophie Lacherade ; Bertrand Fougnie ; Patrice Henry ; Philippe Gamet , Cross Calibration Over Desert Sites: Description, Methodology, and Operational Implementation, IEEE Transactions on Geoscience and Remote Sensing (Volume: 51, Issue: 3, March 2013)

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5. Specific Validation Needs

5.1. Coordination of the Validation Process

- Agreements on essential or standard reference data for validation: Fiducial Reference Measurements (FRM) are reference measurements with known and documented data quality, for which all metadata needed for correlative evaluation are available.
- Harmonisation of validation measurements between the different geographical areas covered by the GEO-AQ constellation => common measurement protocols, common QA protocols, common data format etc.
- Need for appropriate handling of data representativeness (differences in horizontal resolution, differences in geographical/temporal sampling, point-to-area and area-to-volume conversions…)
- Need for harmonised data policy and access to GEO-AQ databases and validation data bases
- Value of deriving child products of GEO-AQ data to encourage e.g. spontaneous validation studies
- Need for enhanced and sustained interactions between satellite and validation measurement experts, validation teams, and algorithm groups
- Need for cal/val best practices, to be endorsed by a representative subset of the CEOS community, addressing end-to-end traceability of the cal/val process,

5.2. Validation of Inter-mission Consistency

- Direct comparison of temporal and spatial averages of L2 products. E.g. for NO_2 , SO_2 and HCHO the observed background levels should be the same. For ozone, averages across common latitude ranges should be comparable.
- Comparison of L2 products with reference measurements from ground based instruments with traceable inter-instrument calibration. The Aeronet and Pandonia networks emphasize homogeneous calibration of instrumentation and will provide reference data for O_3, NO_2, SO_2 and HCHO and aerosol, on a systematic basis.
- Campaigns covering the spatial domains of more than one GEO-AQ mission. Airborne imaging spectrometers will play a pivotal role in providing an inter-domain travelling standard. The consistency of ground based reference measurements can be ensured by exchanging ground based instruments and by dedicated inter-calibration efforts preceding the campaigns (such as the CINDI campaigns for max-DOAS instrumentation). Coordinated campaigns with exchange of instrumentation, of fully joint campaigns, continue the efforts such as KORUS-AQ, partnerships on DISCOVER-AQ.
- Evaluation of GEO-LEO collocated L2 products. The LEO missions are used as a travelling standard. Perfect sun-satellite geometry matching of the LEO measurement with geostationary observations, except for GEMS observations near the equator. However, a large number of measurements with similar Solar Zenith Angles (SZA) is expected to be available. In the beginning of the missions analysis will focus on relatively simple scenes (clear sky, horizontally homogeneous cases, less slant geometries) with comparable surface characteristics.

- Comparison of L1b Solar irradiance. Solar irradiance measurements are directly comparable; differences are expected to reveal mismatches in radiometric and spectral calibration, when changes in solar activity, distance to the sun, and Doppler shifts are accounted for.

- Comparison of L1b Earth radiance and reflectance for well characterised scenes such as bright clouds and dark ocean or desert site used for vicarious calibration. Approaches brightest/darkest targets or radiometric calibration sites can be limited by the low number of such measurements and imperfect knowledge of the targets. Another approach relies on inter-comparisons with the LEO missions that are used as travelling standard exploiting e.g. precise ray matching and approximate ray matching techniques as explored by [Doelling et al., 2013]. Assessment of the inter-mission radiometric consistency and derive radiometric correction terms in coordination with the GSICS initiative.

5.3. Scope and Domains

- Temporal coverage of diurnal cycle and seasonal cycle (cover range of important parameters: SZA, atmospheric temperature, snow/ice cover, surface BRDF…)

- Spatial coverage of the geographic Coverage areas

- Coverage of the driving scenarios (eg NOx limited vs VOC limited chemical regimes for ozone, background conditions vs polluted conditions)

- initial validation during E1, burst mode campaigns at beginning of E2, subsequently systematic validation activities, additional validations campaigns triggered by reprocessing, new products, of satellite datasets over lifetime and beyond, with subsequent (delta-)validations of algorithm and data improvements

5.4. Continuity

- Need for structural funding of validation/monitoring activities (best effort basis fine only during CP when scientific motivation of external partners is high)
- Need for sustainable Cal/Val infrastructure, difficulty to fund campaigns on the long term
- Issue of Cal/Val funding by national agencies and institutions, who often regard validation as a subaltern activity; better chance to get such funding if part of a geophysical investigation/campaign
- Value of tandem operation of a satellite and its successor over at least 6 months/1 year

5.5. New Infrastructure or Approaches

- Validation sites to support LEO+GEO comparison of L2 products
- Characterisation of radiometric calibration sites (such as used for Seviri vicarious calibration)
- Bridge gap between scales of satellite and correlative measurements
- Explore approaches to evaluation of collocated GEO-LEO observations: eg geometry matching

ANNEX A: Geophysical Validation Infrastructure

List below is included mainly in order to identify what could be commonly used for all geo-AQ missions

A.1 Existing Instrumentation

A.1.1 Airborne Instrumentation

- imaging spectrometers (e.g. APEX Airborne PRISM Experiment, AirMAP, Tropolite, Small Whiskbroom Imager for trace gases monitoriNG (SWING), …)
- HALO instrumentation,
- UAV instrumentation,
- in-situ sensors,
- (max-)DOAS, …

A.1.2 Baloon-borne Instrumentation

- Electrochemical ozonesondes (ECC preferred where available): tropospheric and stratospheric (up to about 30 km) vertical profile of O3 partial pressure, convertible to O3 number density using on-board PTU radiosonde measurements of T and water vapour
- PTU radiosonde (various): tropospheric and stratospheric (up to about 30 km) vertical profile of T and water vapour
- NO2 sonde
- AIRCORE?

A.1.3 Ground-based Instrumentation

Ground-based instruments (all fixed, M indicates mobile as well):

- Multi-axis DOAS UV-visible spectrometer (MAXDOAS) (M): NO2 tropospheric column and profile, also SO2, HCHO, BrO, O3, possibly aerosols.
- Zenith-sky DOAS UV-visible spectrometer: stratospheric NO2 and BrO column, O3 total column
- Direct Sun UV-visible spectrometer (M): NO2 and SO2 total column
- FTIR spectrometer: column/profile of O3, CO, CH4, water vapour, also NO2 and HCHO
- Brewer and Dobson UV spectrophotometers (double-monochromator Brewers type Mark-IV preferred where available): O3 total column
- Stratospheric DIfferential Absorption Lidar (DIAL): O3 stratospheric profile
- Tropospheric DIAL: O3 and water vapour tropospheric profile
- Tropospheric Raman lidar: water vapour tropospheric profile
- Aerosol backscatter lidar
- AERONET aerosol sunphotometer
- In situ monitoring: GAW, AGAGE

A.1.4 Other Instrumentation

AirCore, dropsondes

A.2 Networks

A.2.1 Airborne Networks

IAGOS, MOZAIC…

A.2.2 Balloon-based Networks

- Ozonesondes: WMO GAW, NDACC, SHADOZ
- Meteorological radiosonde network

A.2.3 Ground-based Networks

- WMO GAW in situ monitoring network
- WMO GAW contributing ozone column monitoring networks: Brewer, Dobson, UV-visible DOAS, NDACC
- FTIR: NDACC, TCCON
- UV-visible (MAXDOAS, zenith-sky, direct sun): NDACC, PANDORA
- Aerosols: AERONET, EARLINET

A.2.4 Sites

Networks + Cabouw…

A.3 Campaigns

AROMAT,CINDI, Discover-AQ, Korus-AQ, … AROMAPEX

A.4 Other Cal/Val Infrastructures

- Aura Validation Data Center (at NASA-GSFC)
- CEOS Cal/Val Portal
- Cloud/Aerosol/Water/ Radiation Interactions Thematic Center (ICARE, at University of Lille)
- Global Space-based Inter-Calibration System (GSICS)
- Multi-TASTE versatile satellite validation system (at IASB-BIRA)
- Network Of Remote Sensing Ground Based Observation in Support of the Copernicus Atmospheric Service (NORS, at IASB-BIRA)
- NOAA Products Validation System (NPROVS)