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

Prepared by the CEOS Atmospheric Composition Virtual Constellation

and the CEOS Working Group on Calibration and Validation

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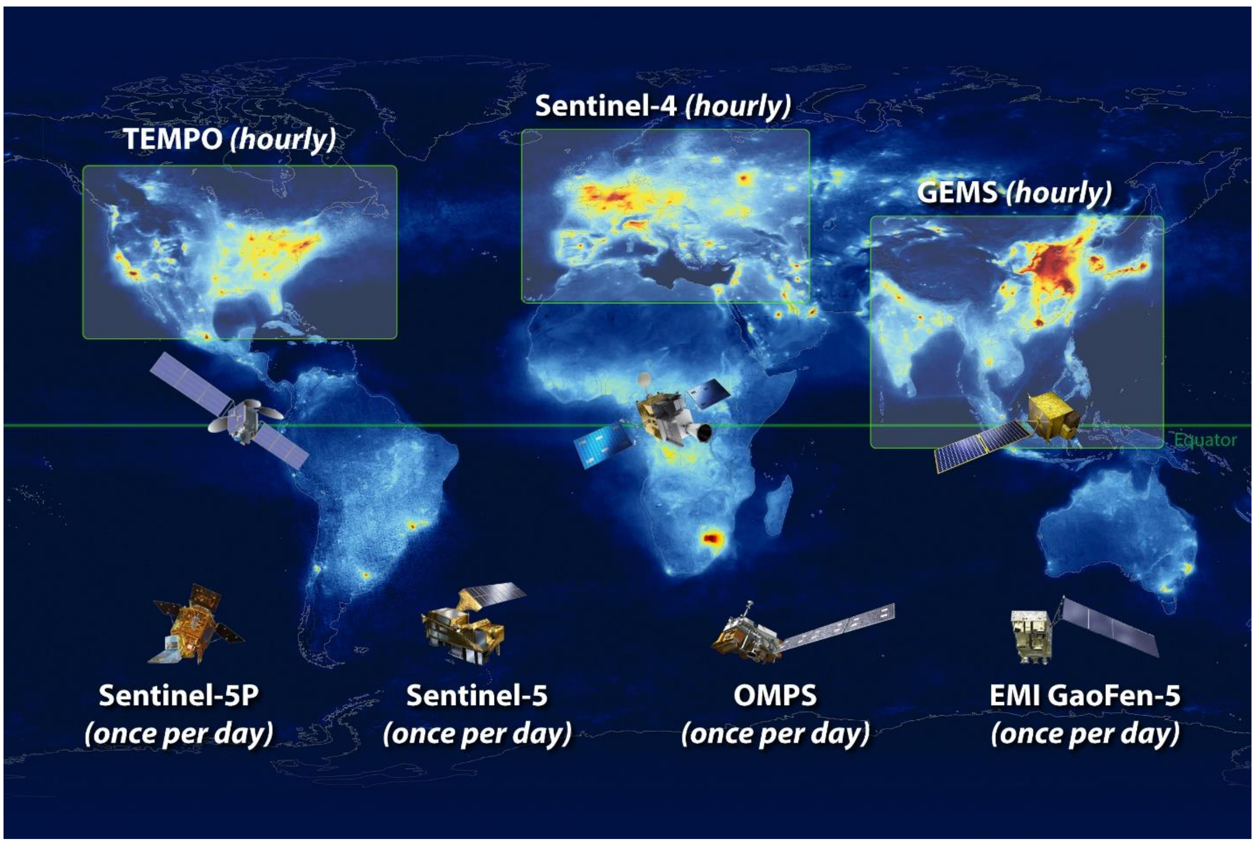

# Table of Contents


Executive Summary ..... 4

Recommendations ..... 5

1. Introduction ..... 6

1.1. Geophysical Validation ..... 7

1.2. New Challenges ..... 9

2. Geo-AQ Missions and Related LEO Missions ..... 11

2.1. GEMS ..... 15

2.2. Sentinel-4 ..... 15

2.3. TEMPO ..... 16

2.4. Sentinel-5 Precursor / TROPOMI ..... 16

2.5. Sentinel-5 ..... 17

2.6. OMPS ..... 17

2.7. EMI ..... 17

3. Product Consistency Across the Constellation ..... 19

3.1. Identification of Constellation Products ..... 19

3.2. Consistency Targets ..... 21

4. Validation Needs ..... 22

4.1. Activities That Need to be Performed Consistently for Each Mission ..... 22

4.1.1. Level-1b Earth Radiance and Solar Irradiance ..... 22

4.1.2. Level-2 Systematic Long-term Validation ..... 22

4.1.3. Total Trace Gas Columns ..... 24

4.1.4. $O_3$ Profile ..... 25

4.1.5. $NO_2$ Tropospheric and Stratospheric Columns ..... 26

4.1.6. $SO_2$ Volcanic Emission Events ..... 26

4.1.7. Aerosol Optical Depth ..... 27

4.1.8. Aerosol Layer Height ..... 27

4.1.9. Emission Source Estimation ..... 27

4.1.10. Recurrent Instruments ..... 28

4.2. Recommendations for Activities Addressing New Geo-AQ Challenges and Inter-mission Consistency ..... 28

4.2.1. Diurnal Cycle Observation Capability ..... 28

4.2.2. Airborne and Mobile Ground-based Sensors as Travelling Standards ..... 30

4.2.3. Inter-mission Radiometric Consistency ..... 31
4.2.4. Inter-mission Consistency of Level-2 Products ..... 31
4.2.5. Level-2 Constellation Products ..... 32
4.3. Coordination and Continuity ..... 33
Reference Documents ..... 34
List of Acronyms ..... 37
Contributors ..... 40
ANNEX: Geophysical Validation Infrastructure ..... 41
A.1 Existing Instrumentation ..... 41
A.1.1 Airborne Instrumentation ..... 41
A.1.2 Balloon-borne Instrumentation ..... 41
A.1.3 Ground-based Instrumentation ..... 41
A.2 Monitoring Networks ..... 43
A.3 Cal/Val Data Archives, Validation Servers, and Other Resources ..... 46

*Cover image: Average tropospheric column $NO_2$ derived from long term measurements made by the OMI instrument on the NASA Aura mission. Graphic: NASA LaRC. $NO_2$ Image: KNMI/ESA.*

## Executive Summary

The Geostationary Air Quality (Geo-AQ) constellation consists of geostationary satellite sensors with a strong focus on air quality. The missions GEMS, Sentinel-4, and TEMPO are currently in preparation and will provide hourly observations of key air pollutants over Asia, Europe, and North America. These geostationary missions will be complemented by a number of low Earth orbiting missions that provide daily global atmospheric composition observations. In the framework of the CEOS AC-VC, coordination and harmonization of the Geo-AQ constellation missions is pursued. The present whitepaper elaborates the validation needs and inter-mission consistency targets for the Geo-AQ constellation.

A set of common products, labelled as 'Constellation Products', is identified, for which inter-mission consistency targets are formulated. This set includes the L1b Earth radiance and solar irradiance products and L2 products for $O_3$, $NO_2$, $SO_2$, HCHO, CHOCHO, and aerosol optical depth. Activities needed to assess and establish this consistency are identified. Recommendations are made for joint validation campaigns with exchange of reference airborne and ground-based instruments, and for the further development of inter-calibration approaches. The main novelty of the Geo-AQ missions, as compared to heritage missions, is the capability of observing the diurnal variation of atmospheric constituents. Recommendations are made for a new type of intensive validation campaign needed to validate this capability.

## Recommendations

1. Consistently perform intensive campaigns dedicated to the validation of the capability of the Geo-AQ missions to observe the diurnal cycle of the target species. Such campaigns are conducted at several supersites within each Geo-AQ mission domain where a comprehensive suite of correlative reference measurements is made and a comprehensive set of auxiliary data from a variety of sources is exploited.

2. Conduct joint validation campaigns with exchange of reference airborne and ground-based instruments.

3. Further develop and eventually apply approaches to the radiometric inter-calibration of the Geo-AQ missions, based on comparisons of Earth radiance data acquired over known targets, SI-traceable test sites where available, precise and approximate ray matching between GEO and LEO pairs of missions, and by taking the LEO missions as a travelling standard. These activities should be pursued within the frame of the WMO GSICS initiative.

4. Further develop and eventually apply approaches to the inter-calibration of the Level-2 products of the Geo-AQ missions. These approaches include the comparison of products with inter-calibrated ground-based network data, cross-validation of Level-2 algorithms by exchanging Level-1b data, comparing zonal mean values of the stratospheric sub-column in the Level-2 ozone products, and taking validated LEO missions as a travelling standard.

5. Systematically process the Level-2 Constellation Products of the Geo-AQ missions, using one selected common algorithm per Constellation Product.

6. Further pursue the harmonization of the reference data used for validation and inter-mission consistency verification of Level-2 products, aiming at common measurement protocols, common QA protocols, common data formats, harmonized data policy and open access.

7. Implement a data centre for storage and exchange of all validation data collected for the Geo-AQ missions. Make these data accessible to the entire community involved in the validation of the Geo-AQ mission products and their inter-mission consistency, very soon after acquisition.

8. Implement a coordinating unit for ensuring the consistency of the approach and the metrics used for validating the Geo-AQ mission products and their inter-mission consistency.

# 1. Introduction

The Atmospheric Composition Virtual Constellation (AC-VC) of the Committee on Earth Observation Satellites (CEOS) strives to coordinate existing and future international space assets and to bring about technical/scientific cooperation and collaboration among space agencies [RD01].

The geostationary atmospheric composition missions Geostationary Environment Monitoring Spectrometer (GEMS, NIER, Republic of Korea), Sentinel-4 (Copernicus/ESA), and Tropospheric Emissions: Monitoring of Pollution (TEMPO, NASA) have a strong Air Quality (AQ) focus and are planned to be launched in the 2019-2023 time frame [RD02]. These missions are distinguished by their capabilities of capturing spectrally resolved radiances in the UV, visible, and for Sentinel-4 also the near infrared spectral domains, with an hourly revisit time. This capability enables the observation of the short lived tropospheric trace gases and aerosol, which are key players for air quality. 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 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 providing similar data products with daily global coverage, including Sentinel-5 (S5) on the Metop-SG series, Sentinel-5 Precursor (S5P), the GOME-2 series on the Metop satellites, the Ozone Mapping Profiler Suite (OMPS) on the Suomi-NPP and JPSS satellites, the Environment Monitoring Instrument (EMI) on the GaoFen-5 satellite, and potentially other future missions. These LEO missions 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. Observations from both LEO and GEO missions will be used to characterise the conditions at validation sites during the acquisition of validation data: multispectral imagers on geostationary satellites (such as the Advanced Baseline Imager (ABI) on GOES-R, the Advanced Meteorological Imager (AMI) on GEO-KOMPSAT-2, or the Flexible Combined Imager (FCI) on MTG-I) bring key information on cloud, aerosol, and surface conditions and on scene heterogeneity; multi-view, multispectral, polarimetric imager data (from LEO sensors such as the Multi-viewing, -channel, -polarisation Imager (3MI) on MetOp-SG, the Directional Polarization Camera (DPC) on GaoFen-5, or the Multi-view Aerosol Mapper (MAP) on the Copernicus candidate mission for anthropogenic $CO_2$ monitoring (CO2M)) offer unique capabilities to distinguish the signatures of surface and aerosol, and provide photon path information for trace gas retrievals.

This document aims at identifying what is needed to validate the data products of the Geo-AQ constellation. The goal is to verify the compliance with user requirements and the inter-mission consistency of the products, in order to enhance the relevance of the mission data for science and policy. While the Geo-AQ missions will also be complemented by the new generation of geostationary meteorological imagers, particularly their capabilities for aerosol and fire characterization, such data products are beyond the scope of this document. The validation of the Geo-AQ products should be coordinated with the validation of products from other mission as far as possible in order to save time and effort and to fully exploit comprehensive validation data sets that are valid for multiple mission.

Section 1 discusses the validation challenges that are either new or specific to the Geo-AQ constellation. A brief overview of the Geo-AQ missions and the above mentioned LEO missions is provided in Section 2. Data products that are common to the Geo-AQ missions are identified and inter-mission consistency targets are formulated in Section 3. Validation needs are identified in Section 4. An inventory of current and planned validation infrastructure is provided in the Annex.

This document has been written by experts of the geostationary AQ missions GEMS, Sentinel-4 and TEMPO, and members of the CEOS AC-VC, the CEOS Working Group on Calibration and Validation (WGCV), and the Global Space-based Inter-Calibration System (GSICS) community. 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 Group on Earth Observations, and the international user community [RD04].

## 1.1. Geophysical Validation

Validation is the process of assessing the data quality by independent means, in a traceable way. This entails a thorough evaluation of the data quality with respect to external reference data, the ex post verification of the theoretical ex ante uncertainties provided by the instrument experts and data producers, and the verification of compliance with key user requirements. The quality of independent data used as a reference must be fully understood and documented, and available with a detailed uncertainty budget. Operationally acquired correlative measurements that are regarded as an essential or standard reference for validation of space-based observations are referred to as Fiducial Reference Measurements (FRM). The GEO-CEOS Quality Assurance framework for Earth Observation (QA4EO) has been established by the WGCV in order to ensure that end-users can easily assess whether Earth Observation data are "fit for purpose" [RD05]. Data products that follow the QA4EO guidelines contain quality indicators that are based on documented and quantifiable assessments of evidence demonstrating the level of traceability to well defined reference standards. 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 before and during the mission lifetime (including mission preparation), and beyond, as outlined below.

### *Pre-launch*

Several validation needs arise already before launch when the space and the ground segment of the mission are being built and integrated:

- On-ground characterisation and calibration campaigns are conducted to verify that the instrument flight models are built according to design, to characterise the instruments, and to generate calibration key data for data processing. Measurement data from these campaigns are needed for functional testing of the Level-1b (L1b) and Level-2 (L2) processors and for routine in flight calibration activities.
- On-ground solar occultation and zenith sky measurements made with the flight models should be considered. Such measurements help to discover instrument anomalies that only become apparent with a stimulus with real high resolution atmospheric signatures and solar irradiance structures, and allow recovery measures e.g. based on dedicated characterisation, calibration, and L2 processing, in time for the start of operations.
- Preparatory activities ensure that all key elements are ready in time for the validation activities in upcoming phases. Depending on the state of the art of validation capabilities, this may include:
    - Development and testing of validation approaches,

- Development and testing of validation data analysis facilities and validation servers,
- Development of instrumentation providing correlative data of FRM quality,
- Inter-calibration of such instrumentation,
- Validation of atmospheric chemistry models and other tools needed to interpret validation data,
- Training and rehearsal validation campaigns.

### *Commissioning Phase (E1)*

The main objective of the Commissioning Phase is to verify, after launch, the health of the mission. This implies functional testing of the instrument, verification of the instrument performance and the operational data processors, consolidation of L1b calibration key data, consolidation of L2 processing key data for, e.g. background corrections, (preliminary) validation of the first L1b and L2 products, and ramp-up of operational validation activities. After acceptance of the space and the ground segments the system is ready for operations. The validation needs in Phase E1 include:

- Early availability of measurement data (L0 and L1b) for timely functional testing and verification of the L1b and L2 processors.
- Early availability of FRM data for initial validation of first L1b and L2 data products.
- Validation of the L1b products including a thorough ex post characterisation of product uncertainties.
- Preliminary validation of the L2 products including an initial characterisation of product quality and properties and an initial ex post verification of ex ante uncertainty estimates.

### *Exploitation Phase (E2)*

The main validation effort is made during the Exploitation Phase in order to determine and maintain the quality of the data products:

- Validation campaigns in the beginning of the Phase E2 are needed for the consolidation of the data processing algorithms and for a thorough ex post characterisation of the product quality and uncertainties. Such activities usually take an intensive effort within a limited period and are based on a comprehensive set of correlative and auxiliary data. A thorough characterisation of the validation scenarios is needed to allow an accurate interpretation of the validation data and of the validation results.
- Follow up validation campaigns later in Phase E2 are needed in order to complement initial validation efforts, to maintain the quality control of existing products e.g. in case of changes in the instrument's behaviour, and possibly to determine the data quality of newly developed products.
- Systematic validation of the key geophysical data products during one year are needed to cover the dynamic range of the products and of their observation conditions such as solar zenith angle, surface albedo, cloud properties, temperature, etc.
- Systematic long-term validation of the key geophysical data products, which will start in Phase E1 and continue throughout the mission lifetime, based on operationally acquired correlative data (FRM and other validation data of appropriate quality). The data handling and evaluation is to a large degree automated, using e.g. an operational validation database and comparison tools for the automated generation of graphs, statistics and reports, responding to user queries. Typically, the systematic long-term geophysical validation is performed by an operational data quality centre running the automated validation data analysis facility and coordinating the interpretation and reporting of the validation results with a dedicated pool of validation and product experts.

The data quality information obtained from these activities needs to be made available to:

- the instrument operators for the verification of instrument health, for the detection of anomalies, for the quantification of degradation, and for the preparation of possible mitigation measures,
- the L1b and L2 teams for the verification of the proper working of the data processors, and for the maintenance and evolution of algorithms,
- the L1b and L2 data users for the correct use of the data.

Re-processing activities may take place periodically during the Phase E2, following calibration key data and/or operational processor algorithm updates, in order to provide a consistent set of mission data consistent with the most recent processing baseline. After each major L2 data reprocessing, adequate validation of the reprocessed data products – referred to as “Delta-validation” of product evolution – needs to be organised.

### *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 and with upgraded retrieval algorithms. Additional re-processing campaigns can be necessary in the longer future to enhance the consistency of the mission data with other long-term data sets. It is vital that metadata, correlative data and analysis tools needed for assessing the mission data quality are stored and kept accessible to users. In this phase, validation activities may include:

- Validation activities after every major re-processing expected to affect the data, in order to verify expected algorithm and data improvements (the so-called ‘Delta-validation’ campaigns),
- Determination of the quality of new data products,
- Evaluation of mission data against user requirements that may have evolved.

## 1.2. New Challenges

The validation approach for the Geo-AQ missions builds on the experience from heritage LEO missions (including GOME, SCIAMACHY, GOME-2, OMI, GOSAT, OCO, 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 validation of air quality satellite observations raises a list of challenges inherent to the large variability of short-lived species and to remote sensing issues at tropospheric altitudes (e.g. RD10, -11). Ongoing validation activities for OMI, S5P and OMPS are already facing such challenges.

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

a) The sampling of the diurnal cycle of atmospheric constituents is a key feature of the Geo-AQ missions and is new with respect to heritage LEO missions. It needs to be demonstrated that temporally varying biases do not dominate the true diurnal variations;
b) Related, the 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. The validation of diurnal cycle observations depends critically on an accurate description of Radiative Transfer (RT). Availability of appropriate directional information on cloud properties, aerosols, surface reflectance and orography is particularly important;

c) The horizontal resolution of trace gas observations has been improved significantly as compared to heritage missions in order to reveal finer spatial structure in the atmospheric composition. The enhanced resolution poses new challenges to the validation, especially for observations near pollution sources, where strong spatial gradients occur. Validation of such observations depends critically on the approach to handling mismatches of spatial representativeness between satellite and 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 are also new effects to be taken into account;
d) The geographic coverage areas of the different geostationary AQ missions do not overlap spatially, which excludes direct inter-comparisons of products. Observations from LEO polar orbiting satellites and from inter-calibrated ground based networks serve as a transfer standard for achieving and monitoring the consistency of the products among the Geo-AQ missions;
e) Obtaining accurate geo-location knowledge is challenging for geostationary sensors. Accurate geo-location knowledge is needed for L2 data processing and data applications, and also for the validation of AQ products. The geo-location performance needs to be validated;
f) Nadir satellite observations provide little information on the vertical distribution; nevertheless, the retrieval sensitivity to several species varies vertically. Therefore, information on the vertical distribution of measured species and their retrieval parameters is important for the validation of AQ missions in general and is particularly important for the Geo-AQ missions given that the vertical distributions can change dramatically through the day due to, e.g., the growth and collapse of the planetary boundary layer.

Since the Geo-AQ missions will provide data products as input to operational services and near real-time applications, additional challenges arise as to the speed of retrieval algorithms and processors, the timeliness and robustness of data processing and delivery, the interoperability of data and metadata formats, the set-up and maintenance of service continuity etc. Several of those challenges of operational and service-oriented nature apply also to the validation activities.

# 2. Geo-AQ Missions and Related LEO Missions

In this section brief mission overviews are provided for the Geo-AQ constellation elements GEMS, Sentinel-4, and TEMPO and for a selection of related LEO missions including 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 Earth Venture Program mission and takes the role of a precursor mission or first element of the atmospheric observational capability of the GEO-CAPE mission. 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 a research-to-operational mission in the GEO-KOMPSAT-2 programme designed to provide operational atmospheric composition data over Asia ultimately.

The three missions are implemented as nadir looking grating spectrometers covering the UV, the visible and, depending on the missions, also the near infrared. Key mission characteristics are listed for the geostationary (Table 2.1) and LEO missions (Table 2.2). The spatial domains of the Geo-AQ missions depicted schematically on the document cover page cover Asia, Europe, and North America and have essentially no overlap. The expected mission lifetimes are shown in Table 3. Amongst the GEO missions, GEMS is expected to be launched first (expected early 2020), followed by TEMPO and Sentinel-4 (a few years later). It is expected that the lifetimes of the three Geo-AQ missions will overlap significantly. Also, it is expected that there is significant temporal overlap with the LEO missions, of which OMPS, Sentinel-5P, and EMI have been launched already. 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 2.1. 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** | Instrument delivered early 2018 Instrument AIT (to S/C) | Detailed Design Phase, CDR completed in 2017 | Instrument delivered fall 2018 |
| **Host satellite** | GEO-KOMPSAT-2B | MTG-S | TBD |
| **Expected Launch** | Early 2020 | 2023 (Flight Acceptance Review of first MTG-S in 2022) | Early 2022 |
| **Payload** | UV-Vis 300-500 nm | UV-Vis-NIR 305-500, 750-775 nm | UV-Vis 293-490, 540-740 nm |
| **Key Products** | $O_3$, $NO_2$, $SO_2$, HCHO, CHOCHO, 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 × 8 km E/W @38N | 8 km × 8 km @45N | 2.1 km N/S × 4.7 km E/W @35N |
| **Nominal product resolution** | 7 km N/S × 8 km E/W @38N (gas), 3.5 km N/S × 8 km E/W @38N (aerosol) | 8.9 km N/S × 11.7 km E/W @45N | 8.4 km N/S × 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 FCI imager on MTG-I w.r.t. aerosol and clouds. | GEO-CAPE precursor. Synergy with GOES-R/S ABI w.r.t. aerosol and clouds. |

*Table 2.2. Key parameters of the LEO missions Sentinel-5P, Sentinel-5, OMPS and EMI.*

| | Sentinel-5P | Sentinel-5 | OMPS | EMI |
|---|---|---|---|---|
| **Orbit (Equator crossing time)** | Low-Earth (13:30) | Low-Earth (09:30) | Low-Earth (13:30) | Low-Earth (13:30) |
| **Domain** | Global | Global | Global | Global |
| **Revisit** | 1 day | 1 day | 1 day | 1 day |
| **Status** | Launched | CDR completed early 2019 | Operational | Operational |
| **Host satellite** | Dedicated platform with one instrument | MetOp-SG A | Suomi-NPP and JPSS series | GaoFen-5 |
| **Expected Launch** | October 2017 | 2022 (Flight Acceptance Review first MetOp-SG A) | 2011 (Suomi-NPP), 2017 (first JPSS) | May 2018 |
| **Payload** | TROPOMI. UV-Vis-NIR-SWIR: 270-500, 675-775, 2305-2385 nm | UV-Vis-NIR-SWIR: 270-500, 685-773, 1590-1675, 2305-2385 nm | Nadir mapper: 0.3-0.38 µm, Nadir profiler: 0.25-0.31 µm, Limb profiler: 0.29-1 µm | UV-Vis-NIR: 240-315, 311-403, 401-600, 590-790 nm |
| **Key Products** | $O_3$, $NO_2$, $SO_2$, HCHO, CO, $CH_4$, aerosol, surface UV | $O_3$, $NO_2$, $SO_2$, HCHO, CHOCHO, CO, $CH_4$, aerosol, surface UV | $O_3$, $NO_2$, $SO_2$, aerosol (nadir mapper), $O_3$ (nadir/limb profiler) | $O_3$, $NO_2$, $SO_2$, HCHO, aerosol |
| **Spatial Sampling** | 28×7 $km^2$ in the UV-1, 3.5×7 $km^2$ in the UV-2 to NIR, 7×7 $km^2$ elsewhere, @nadir | 7 km × 7 km @nadir | 13 km × 17 km (nadir mapper), 50 km × 50 km (nadir profiler), @nadir | 48 km × 13 km |
| **Nominal product resolution** | See above | 7 km × 7 km @nadir | 50 km (S-NPP mapper), 17 km (JPSS mapper), 250 km (S-NPP profiler), 50 km (JPSS profiler), @nadir | 48 km × 13 km |
| **Notes** | In formation with S-NPP for synergy with VIIRS imager and CrIS sounder (for cloud and $O_3$ information). | Three instruments in sequence on MetOp-SG-A. Synergy with IASI-NG sounder, MetImage and 3MI imagers on same platform. | Four instruments in sequence on S-NPP, JPSS-1, -2, -3. Synergy with VIIRS imager and CrIS sounder on same platform. | Synergy with Atmospheric Infrared Ultraspectral (AIUS), Directional Polarization Camera (DPC), and Greenhouse-gases Monitoring Instrument (GMI). |

***Table 2.3. Expected mission lifetimes of the Geo-AQ missions (red) and the complementing LEO missions (blue). TEMPO prime mission of approximately 2 years can be followed by multiple 2-year extensions as long as the instrument remains healthy.***

| 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 | | | | | | | | | | | | | | | |

## 2.1. GEMS

The objective of the Korean Geostationary Environment Spectrometer (GEMS) mission (http://www.nier.go.kr; Choi et al. 2019 (RD12); Kim et al. 2019 (RD13)) is to provide observations of tropospheric composition over Asia at high spatial and temporal resolution, thus contributing to the establishment and implementation of a science-based policy for air quality. The GEMS instrument is on-board the GEO-KOMPSAT-2 series of the Korea Aerospace Research Institute (KARI), which includes the Advanced Meteorological Imager (AMI) and the Geostationary Ocean Color Imager (GOCI-2). The GEMS instrument covers the spectral range 300-500 nm with a spectral resolution of 0.6 nm, and has a revisit time of one hour within the target area (Asian region; 5°S – 45°N & 75°E-145°E) with a spatial resolution of 7×8 $km^2$ at Seoul. The key products of the GEMS mission are $NO_2$, $O_3$, HCHO, CHOCHO, $SO_2$, aerosols, UV index, and cloud and surface properties.

KARI and Ball Aerospace have completed the development and environmental testing of the GEMS instrument and the instrument was delivered to KARI for system integration in February 2018. The L1 processor was delivered by industry (BATC) to KARI, and L2 processor was developed by universities and delivered to NIER. The expected launch date of GEO-KOMPSAT-2 is early 2020, and the expected lifetime is 10 years after launch.

NIER are considering issuing an Announcement of Opportunity for Phase E1 geophysical validation about 1 year before launch following the ESA S5P approach.

## 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) embarked on the geostationary Meteosat Third Generation-Sounder (MTG-S) platforms (http://www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Sentinel-4_and_-5; Ingmann et al. 2017 (RD14); ESA Special Publication SP-1334 (RD15)). Key features of the S4/UVN instrument are the spectral range from 305 to 500 nm with a spectral resolution of 0.5 nm, and from 750 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 has 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 L2 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 L1b prototype processor is in the detailed design phase since completion of the Critical Design Review in 2017. The Critical Design Review of the L2 processor development has been completed early 2019 with a first version of the algorithm breadboarding and an independent verification. The expected launch date of the first MTG-S satellite is 2023, 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 six months is scheduled after launch. EUMETSAT will operate the S4/UVN instruments and will process the mission data up to L2.

It is envisaged that an ESA Announcement of Opportunity for Phase E1 geophysical validation will be issued about 1.5 years before launch following the S5P approach. In addition EUMETSAT will initiate the required preparation for operational calibration and validation activities which will start in Phase E1 and continue throughout Phase E2.

## 2.3. TEMPO

The Tropospheric Emissions: Monitoring of Pollution (TEMPO; http://tempo.si.edu, Zoogman et al. 2017 (RD16)) satellite instrument will measure atmospheric pollution and much more over North America, ranging from Mexico City to the Canadian oil sands, and from the Atlantic to the Pacific. Its high temporal resolution (hourly or better in daylight, with selected observations at 10 minute or better sampling) and high spatial resolution (10 $km^2$ at the centre of the field of regard) resolves pollution sources at sub-urban scale, improves emission inventories, monitors population exposure, and enables effective emission-control strategies. TEMPO will measure $O_3$ profiles (including boundary layer $O_3$), $NO_2$, $SO_2$, HCHO, CHOCHO, $H_2O$, BrO, IO, and HONO, as well as clouds and aerosols. Applications include: intercontinental pollution transport; biomass burning and $O_3$ production; aerosol products including synergy with GOES infrared measurements; lightning $NO_x$; soil $NO_x$ and fertilizer application; crop and forest damage from $O_3$; chlorophyll and primary productivity; foliage studies; halogens in coastal and lake regions; ship tracks and drilling platform plumes; water vapor studies including atmospheric rivers, hurricanes, and corn sweat; volcanic emissions; high-resolution pollution versus traffic patterns; tidal effects on estuarine circulation and outflow plumes; and air quality response to power blackouts and other exceptional events. The instrument has been delivered and will be integrated on a telecommunication satellite that will be launched in early 2022 to a geosynchronous orbit near 90° West.

As an Earth Venture project, the TEMPO mission includes validation of baseline $O_3$, $NO_2$, and HCHO products. It is envisaged that a NASA Announcement of Opportunity for an expanded TEMPO science team, including additional validation activities, will be issued after successful TEMPO launch.

## 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 Service (CAMS) and Climate Change Service (C3S). The Sentinel-5 Precursor mission comprises the TROPospheric Monitoring Instrument (TROPOMI) carried on board a dedicated, near polar orbiting platform (http://www.tropomi.eu; Veefkind et al. 2012 (RD17), ESA Special Publication SP-1332 (RD18)). 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 is 28 km in the UV-1, 3.5 km in the UV-2 to NIR, and 7 km at other wavelengths. The mission is 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 product for cloud properties.

The Sentinel-5 Precursor mission was launched in October 2017. The expected lifetime is 7 years.

Operational validation of the S5P data products is performed through the Validation Data Analysis Facility (VDAF) of the S5P Mission Performance Centre (MPC). Complementarily, ESA released a CalVal Call for the international S5P Validation Team in 2014. The Sentinel-5p Scientific Validation Implementation Plan [RD09] was established based on over 50 proposals received in response to this call. Operational validation and scientific validation activities are on-going.

## 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 (http://www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Sentinel-4_and_-5; Ingmann et al. 2017 (RD14); ESA Special Publication SP-1336 (RD19)). The S5/UVNS instrument covers the ultraviolet (270-370 nm), visible (370-500 nm) near-infrared (685-710 & 745-773 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, CHOCHO, $CH_4$, CO, aerosols, and spectral UV solar irradiance.

The development of the S5/UVNS instruments and the L1b prototype processor is currently in the detailed design phase and the Critical Design Review was completed early 2019. The Critical Design Review of the L2 processor development is expected to be completed mid 2019. The expected launch date of the first Metop-SG satellite A is 2022, 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 six months is scheduled after launch. EUMETSAT will operate the S5/UVNS instruments and will process the mission data up to L2.

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. In addition EUMETSAT will initiate the required preparation for operational calibration and validation activities which will start in Phase E1 and continue throughout Phase E2.

## 2.6. OMPS

OMPS, the Ozone Mapping and Profiler Suite, will continue the US program for monitoring the Earth's ozone layer by using advanced hyperspectral instruments that measure ultraviolet and visible backscattered radiance from the Earth's atmosphere and also make periodic measurements of the solar irradiance (https://jointmission.gsfc.nasa.gov/omps.html; https://www.jpss.noaa.gov/omps.html; Flynn et al. 2006 (RD20)). The first OMPS was launched into a 13:30 sun-synchronous orbit on the Suomi National Polar-orbiting Partnership (S-NPP) satellite in 2011, the second OMPS followed in 2017 on the Joint Polar Satellite System (JPSS-1 renamed NOAA-20 in orbit). Three more JPSS satellites will be launched between 2022 and 2031. OMPS is a three-instrument suite. The nadir mapper measurements (~200 channels from 300 to 380 nm at 1 nm FWHM resolution) provide estimates of total column ozone with daily global coverage of the sunlit Earth at 50 km ground-resolution (17 km for NOAA-20 and future instruments) as well as reflectivity, aerosol and $SO_2$ products. The nadir profiler measurements (~50 channels from 250 to 310 nm at 1 nm FWHM resolution) provide estimates of the vertical distribution of ozone in the middle and upper stratosphere. The limb profiler provides measurements (from 290 to 1000 nm with varying resolution for 100 limb tangent heights from 10 to 90 km) to estimate ozone in the lower stratosphere and troposphere with high vertical resolution. The limb profiler is not present in the OMPS on NOAA-20 but will return on JPSS-2.

## 2.7. EMI

The objective of the Environment Monitoring Instrument (EMI) is to measure trace gases such as $NO_2$, $SO_2$, and $O_3$. The EMI instrument flies on board the Gaofen-5 (GF-5) satellite as part of the Chinese civilian remote sensing satellite program Gaofen. The payload of GF-5 includes, next to EMI, the Advanced Hyperspectral Imager (AHSI), the Visual and Infrared Multispectral Sensor (VIMS), the Greenhouse-gases Monitoring Instrument (GMI), the limb sounder Atmospheric Infrared Ultraspectral (AIUS), and the Directional Polarization Camera (DPC). G-5 has been launched in 2018 and has a design lifespan of 8 years.

# 3. Product Consistency Across the Constellation

The success of the Geo-AQ missions depends critically on the traceable quality of the data products and, in particular, the consistency of products across the missions. The validation activities should therefore support a traceable assessment and ideally enhancement of this consistency. In Section 3.1, constellation products are identified as geophysical parameters that are common to the product portfolios of the Geo-AQ missions. In Section 3.2, inter-mission consistency targets for the constellation products are established. Activities aiming at the verification of inter-mission consistency are outlined in Section 4.2.

## 3.1. Identification of Constellation Products

The common products of the Geo-AQ and complementing LEO missions include the L1b Earth radiance and solar irradiance products and the L2 products for $O_3$, $NO_2$, $SO_2$, HCHO, CHOCHO, the UV aerosol index, and aerosol and cloud characteristics (see Table 3.1):

- 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 2.1). The LEO instruments also cover this range fully (S5, S5P) or partly (up to 380 nm for the OMPS nadir mapper, Table 2.2). L2 products are derived from reflectance (or sun-normalised radiance), benefitting from a partial cancellation of radiometric calibration errors. The common spectral ranges of Earth radiance, solar irradiance and reflectance are considered as Constellation Products.
- The trace gas total column densities for $O_3$, $NO_2$, $SO_2$, HCHO, and CHOCHO are Constellation Products. Additionally, total columns generated using a commonly agreed retrieval approach should be considered. Dedicated processing of such Constellation Products with common algorithms or with consistent algorithm settings (degree of polynomial, treatment of interfering species, fit window, etc.) would facilitate the evaluation of collocated observations by LEO and GEO missions.
- The vertical sensitivity of the ozone profile depends on the spectral range used in the retrieval scheme. The TEMPO, GEMS, and Sentinel-4 algorithms all exploit the ozone absorption signatures in the Hartley and Huggins bands in the UV spectral range. These signatures allow tropospheric and stratospheric sub-columns to be discerned and bring information on the lower tropospheric (0-6 km) sub-column, but offer little sensitivity to near surface ozone. The TEMPO algorithm also exploits the ozone absorption signature in the Chappuis band in the visible spectral range, which is sensitive to near surface ozone. The lower boundaries of the spectral ranges in the UV limit the stratospheric profile information (especially for Sentinel-4). The stratospheric and tropospheric sub-columns are Constellation Products. Additionally, the lower tropospheric sub-column can be considered, in view of its importance for air quality applications. The ozone profile is observed by various nadir IR sounders, including the geostationary IRS on MTG and the LEO sensors CRiS, IASI, and IASI-NG. IR based ozone products are complementary to UV-visible based products in view of the vertical sensitivity profile and offer common profile information e.g. in the free troposphere. The IR profile information in this common vertical range should be used as a validation means for, or even as a contribution to, the Geo-AQ ozone profile constellation product.
- The $NO_2$ products contain, in addition to total columns, also tropospheric and stratospheric 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 atmospheric chemistry models. Nevertheless, the tropospheric $NO_2$ sub-column is considered as a Constellation Product in view of its importance for air quality applications.

- Although the Geo-AQ missions are not dedicated aerosol missions, aerosol products like the Aerosol Optical Depth (AOD) might be considered as a Constellation Product. The comparability of AOD data might be limited by differences in the treatment of surface and cloud characteristics and in the assumptions made on aerosol microphysics. The L2 product portfolio of S4, S5 and S5P covers the Aerosol Layer Height (ALH) derived from measurements in the $O_2$-A band, which contributes also to the AOD product. A similar product might also be developed for EMI which also covers this spectral domain. GEMS and TEMPO may use information from the UV and from advanced meteorological sounders, AMI and ABI, to improve estimation of aerosol height and thereby improve intermission commonality of AOD products. The ALH might be considered as a constellation product.
- The UV Absorbing Aerosol Index (UVAI) is mainly used to detect elevated absorbing particulates and is strictly speaking not a geophysical parameter. Quantitative comparisons of UV Absorbing Aerosol Index (UVAI) data are difficult since the index depends on many scene parameters at the same time (including the spectral aerosol absorption, aerosol amount, elevation and spectral surface reflectance, etc.). Therefore, the UVAI is not considered as Constellation Product.
- The cloud products are generated mainly as auxiliary products for the trace gas and aerosol retrievals and are not considered as Constellation Products.
- It is expected that measurements from the IRS on MTG will be used for atmospheric composition observation exploiting also the sensitivity to CO, $NH_3$ (not covered by the current L2 product portfolio), $O_3$, dust and ash. These air quality relevant species are also observed by various LEO missions including S5 and S5P (using the SWIR) and the nadir IR sounders CRiS, IASI, and IASI-NG. These products could be considered as constellation products in the future.

***Table 3.1. Constellation Products 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 | |
| $O_3$ profile | Stratospheric and tropospheric sub-columns | Differences in averaging kernels need to be accounted for. A sub-column covering the lower troposphere should be considered. |
| $O_3$ total column | Slant and vertical columns | Additionally, total columns based on a commonly agreed retrieval approach should 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 | |
| CHOCHO 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. |
| AOD total column | Matching pairs of reference wavelengths (S4: 342, 368, 417, 443, 457 nm; TEMPO: 354 and 388 nm; GEMS: 443 nm) | Different approaches for surface reflectance, aerosol microphysics, and aerosol layer height must be considered. |

## 3.2. Consistency Targets

For the Constellation Products identified in Section 3.1, consistency targets have been developed over the past two years by AC-VC members (http://ceos.org/meetings/ac-vc-13/, http://ceos.org/meetings/ac-vc-14/). Consistency targets (Table 3.2) account 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 3.2. Constellation products and target limits of systematic differences.***

| Level-2 Product / Parameter | | Maximum allowed Systematic difference |
|---|---|---|
| $O_3$ | Total column | 1% |
| | Stratospheric column | 5% |
| | Tropospheric column | 20% |
| | Lower tropospheric (0-6 km) column | No target is identified. The consistency needs to be assessed. |
| $NO_2$ | total column | $1\times10^{15}$ molec/cm$^2$ |
| | tropospheric column | $1\times10^{15}$ molec/cm$^2$ |
| $SO_2$ total column | | $1\times10^{16}$ molec/cm$^2$ |
| HCHO total column | | $1\times10^{16}$ molec/cm$^2$ |
| CHOCHO total column | | $4\times10^{14}$ molec/cm$^2$ |
| AOD total column | | 0.05 @ 440 nm |
| Level-1b Earth radiance | | 2-5% |
| Level-1b solar irradiance | | 1-2% |
| Reflectance | | 2-5% |

# 4. Validation Needs

This section describes what is needed in order to address the challenges outlined in Section 1, and ultimately to enhance the relevance of the Geo-AQ mission data for science and policy. Section 4.1 specifies validation activities that are considered necessary, based on experience from heritage missions, and that need to be performed consistently for each individual mission. Section 4.2 makes specific recommendations addressing new challenges specific to the geostationary AQ mission class aiming at the verification and enhancement of the inter-mission consistency. Needs related to the coordination and continuity of the validation process are stated in Section 4.3.

## 4.1. Activities That Need to be Performed Consistently for Each Mission

### 4.1.1. Level-1b Earth Radiance and Solar Irradiance

A solid validation and good knowledge of the L1b data quality is necessary before these data can be released and L2 data product validation can be started. Systematic long-term monitoring of the Earth radiance and solar irradiance products is necessary to maintain the data quality (to determine degradation, analyse and mitigate anomalies, keep calibration key data up to date, tune the setting of quality flags, etc.). The core activities covering verification, validation, and data quality management are typically performed by a Mission Quality Team, and are not elaborated in this document. Activities needed to assess the inter-mission consistency of L1b products are discussed in Section 4.2.3.

### 4.1.2. Level-2 Systematic Long-term Validation

Long-term systematic validation of the L2 products is typically performed by a Mission Quality Team and starts during the Phase E1 once L1b data become available. It is based on comparisons of satellite data with reference data from operational networks of inter-calibrated ground-based instruments (Fiducial Reference Measurements and other validation data sources, Table 4.1) and relies on auxiliary information that is generated or acquired operationally and that is available with high reliability including e.g. meteorological data from numerical weather prediction models and trace gas and aerosol data from atmospheric chemistry models.

Ideally, the long-term systematic validation covers all key output parameters of all products in the full dynamic range of product values and relevant influence quantities (e.g. pollution level, atmospheric state, sun-satellite geometry, surface characteristics, etc.). In practice, the finite number of operational network stations and availability of auxiliary data pose limitations. Dedicated validation activities (see subsequent sections) are needed to complement the long-term systematic validation.

In the past, ozone product validation relied mainly on Brewer/Dobson daily mean, DOAS/UV-visible twilight observations, and near-noon ozonesonde launches. Hourly ground-based observations should be enhanced and used to validate the hourly products from the geostationary sensors.

***Table 4.1. Fiducial Reference Measurements and other validation data for Level-2 systematic long-term validation.***

| Product | Ground-based remote sensing | In situ |
|---|---|---|
| Ozone total column | Direct sun and scattered light (MAX-DOAS and ZSL-DOAS) spectrometer measurements (e.g. from Brewer, Dobson, SAOZ/DOAS (NDACC) and Pandora (PGN)) | |
| Ozone profile | Stratospheric and tropospheric ozone lidars (e.g. NDACC and TOLNet), millimetre wave radiometers, FTIR | Balloon-borne electro-chemical cell ozonesondes, ground stations (for the near-surface partial column) [1)] |
| $NO_2$ total, tropospheric and stratospheric columns | Direct sun spectrometer measurements for total $NO_2$ and scattered light measurements (MAX-DOAS and ZSL-DOAS) for tropospheric and stratospheric $NO_2$, (e.g. from DOAS (NDACC) and Pandora (PGN)) | |
| $SO_2$ total column | Direct sun and scattered light (MAX-DOAS) spectrometer measurements (e.g. from Brewer and Pandora (PGN) [2)]) | |
| HCHO total column | Direct sun and scattered light (MAX-DOAS) spectrometer measurements (e.g. from DOAS (NDACC) and Pandora (PGN) [2)]) | Proxy for tropospheric column from ground-based in-situ measurements [2)] complemented by boundary layer height estimates |
| CHOCHO total column | Direct sun and scattered light (MAX-DOAS) spectrometer measurements (e.g. from DOAS (NDACC) and Pandora (PGN)[2)]) | |
| Cloud (Top) Height, Cloud Optical Thickness | Radar/lidar measurements (e.g. from CLOUDNET) | |
| AOD | Direct sun and scattered light measurements (e.g. from sun-photometers (AERONET), and Pandora (PGN)[2)]) | |
| Aerosol Layer Height | Lidar (e.g. from EARLINET, MPLNET, ADNET), ceilometers (e.g. from E-PROFILE) | |

[1)] mainly for the TEMPO product which offers sensitivity to near surface ozone.

[2)] product development ongoing/planned, not yet operational.

### 4.1.3. Total Trace Gas Columns

Dedicated efforts are needed to validate the total column trace gas products ($O_3$, $NO_2$, $SO_2$, HCHO, CHOCHO) based on comprehensive reference and auxiliary data sets, including also data that cannot be acquired on a long-term systematic basis (e.g. airborne measurements). For the validation of the total column products using reference data from ground based remote sensing instrumentation, the following auxiliary data are needed:

- Trace gas profiles: The retrieval sensitivity decreases toward the ground due to light scattering in the atmosphere for the above-mentioned products, but especially for products with fit-windows at short wavelengths ($O_3$ and $SO_2$). The handling of the sensitivity profile is an essential part of the retrieval scheme and is usually implemented based on the Air Mass Factor (AMF) concept. For the AMF computation, assumptions are made regarding trace gas profile shapes, and a-priori information on surface reflectance and clouds is used. For ozone, ozonesonde and lidar measurements are the preferred source of profile data. For $NO_2$, in-situ measurements from aircraft and balloon sondes are the preferred source of profile data. If such in-situ profile data is unavailable, profile information from atmospheric composition models or from the reference ground based remote sensing instrumentation might be considered.
- Aerosol characteristics: In many operational algorithms the impact of aerosol on the AMF is accounted for implicitly, relying on cloud parameters from L2 products. In this case, a dedicated analysis is needed to verify the approach of treating aerosol as cloud. For this purpose, reference aerosol data from ground based sun-photometers or from dedicated aerosol satellite instrumentation should be used.
- Surface characteristics: recent estimates for the surface reflectance and its spectrally resolved bi-directionality should be considered if available and if considered more accurate than the (typically climatological Lambertian equivalent) albedo data used in the retrievals. Effects on cloud retrievals might be particularly important.
- Cloud parameters: cloud characteristics from meteorological imagers and from ground based networks of ceilometers, radars and lidars should be used for cloud screening and for the validation of the cloud retrievals (cloud fraction, top height and optical thickness). Cloud characteristics from meteorological imagers are a good reference as input to cloud correction if not already exploited by the retrieval schemes.

It is expected that a number of campaigns are needed to collect such comprehensive validation data sets, and cover the relevant ranges of quantity values (from minimum to maximum with good sampling in between) and influence quantities. The validation needs to cover the full range of sun-satellite geometries (including very slant illumination and viewing angles) for all products. The validation needs also to consider the full range of surface albedo values and combinations of surface/cloud properties. For ozone, very large and very low total ozone columns that may occur (up to 600 DU and down to 100 DU), with enhanced gradients and variability especially during springtime, should be covered. For HCHO and CHOCHO the validation data should cover a broad variety of cases with various precursor types (volatile organic compounds) from various sources (biogenic, biomass burning or anthropogenic) and with different lifetimes.

Analyses with dedicated tools are needed to understand the apparent differences between satellite and ground-based reference measurements and to quantify the contributing measurement errors and representativeness errors. The impact of co-location mismatches and differences in the respective sensitivities can be estimated based on atmospheric composition models and on forward observation operators for both satellite and ground-based reference measurements (Verhoelst et al. 2015 (RD21)). A dedicated effort is needed to establish the forward operators and the computation of representativeness errors. Eventually, it might be possible to generate such error and consistency diagnostics systematically in data assimilation systems where both the satellite and the reference data are assimilated using fully descriptive (3-D) observations operators.

The validation of the $SO_2$, HCHO, and CHOCHO products is challenging since the signature in satellite data tends to be weak and dominated by radiometric errors. In background and anthropogenic pollution conditions, the trace gas burden is usually low and the bulk of the load is located in the boundary layer where the retrieval sensitivity is weak (especially for $SO_2$). Aggregated validation data need to be evaluated in order to obtain meaningful results.

Biases related to instrument effects need to be assessed using total column data that are re-evaluated using the reference trace gas profile data.

The timely availability of correlative and auxiliary data is important for a fast identification of possible anomalies in the satellite data.

#### 4.1.4. $O_3$ Profile

The ozone profile products differ from mission to mission as the vertical sensitivity of a retrieval depends on the available spectral ranges and the actual sensor performance. The TEMPO product exploiting the Chappuis band in addition to the UV spectral range is sensitive to near surface ozone. The GEMS and Sentinel-4 algorithms relying only on the UV spectral range are sensitive to the lower tropospheric (0-6 km) sub-column but less to near surface ozone. GEMS and TEMPO yield more stratospheric profile information as compared to Sentinel-4, since the latter does not cover wavelengths below 305 nm. All missions provide profile information with several degrees of freedom of signal, sufficient to separate stratospheric and tropospheric sub-columns.

The validation of the ozone profile products is based mainly on comparisons with ozonesonde observations which are made routinely. Ozonesondes offer high vertical resolution, typically 100 m. The agreement with the satellite profiles needs to be evaluated statistically, both directly after mass conservative re-gridding and indirectly after applying the vertical averaging kernels of the satellite retrieval to the sonde data.

Comparisons to state-of-the-art atmospheric composition models are needed to complement the sonde-based validation, since ozonesonde measurements are usually made only once a week or even less frequently. Additionally, ozonesondes are usually coupled to a meteorological PTU sonde and thus launched at the time recommended for WMO’s Upper-Air Global Observing System. Model data can help to confirm the performance of the ozone profile products over the diurnal cycle. Also, data obtained during field campaigns can be especially useful because ozonesondes can be launched multiple times within a single day to obtain validation data over the diurnal cycle.

The tropospheric profile information can be verified using reference data from instrumentation on commercial aircrafts through the IAGOS programme. The IAGOS-CORE and IAGOS-CARIBIC instrument packages provide regular profile measurements of ozone, water vapour and other trace gases during take-off and landing at several airports in Europe and on other continents.

Brewer and Dobson Umkehr measurements and MAX-DOAS measurements provide ozone profile information, although at a very limited vertical resolution, range and sensitivity. In any case, averaging kernels of both observation systems need to be accounted for in order to reduce comparison errors due to significant differences in vertical smoothing.

Ground-based ozone lidar instruments provide useful reference profiles in the troposphere or the stratosphere, depending on their settings. With those higher vertical resolution instruments (compared with Umkehr and MAX-DOAS), comparison errors associated with vertical smoothing issues are caused mainly by the satellite data, for which availability of the vertical averaging kernels and a-priori information is thus necessary. As discussed in the previous section, dedicated analyses are needed to understand the apparent differences between satellite and ground-based reference measurements and to quantify the contributing measurement errors, co-location mismatch errors and representation errors.

Observations from limb sounders offer high vertical resolution and can be considered as a reference for the stratospheric profile shape, for the validation of the stratospheric ozone data from the nadir sounders. It is expected that OMPS-Limb data will be available when the Geo-AQ missions are being launched, as well as profile data from future limb sounders like ALTIUS. Possibly also data from existing limb sounders may be still available (e.g. from Aura MLS, Odin OSIRIS and SMR, Scisat-1 ACE-FTS, SAGE-III ISS).

### 4.1.5. $NO_2$ Tropospheric and Stratospheric Columns

Nadir satellite based measurements are sensitive to the total $NO_2$ column amount and provide only limited information regarding the vertical distribution. Tropospheric and stratospheric sub-columns are reported separately in the products. The separation is usually based on a reference sector (usually over parts of the Pacific Ocean assumed to be free of $NO_2$) or a forecast profile data that is obtained by data assimilation and spatial filtering techniques. The stratospheric $NO_2$ information should be validated as a stand-alone product, and not only as a corrective term for deriving tropospheric column from total column.

Correlative data

- tropospheric $NO_2$: ground-based MAX-DOAS UV-visible spectrometers
- total $NO_2$: ground-based direct Sun UV-visible spectrometers (e.g. of the Pandora type)
- total $NO_2$ in pristine areas and stratospheric $NO_2$: ground-based twilight measurements acquired by zenith-scattered-light DOAS UV-Visible spectrometers, with support from a 1D stacked-box photochemical model to account for diurnal variation effects
- stratospheric $NO_2$ profile measurements from limb/occultation
- stratospheric modelling data

### 4.1.6. $SO_2$ Volcanic Emission Events

Volcanoes can emit large amounts of $SO_2$ that are transported over large distances in elevated plumes. The signatures of elevated volcanic $SO_2$ in satellite observations can be very strong especially for eruptive events. Owing to their improved spatial resolution, new sensors are also able to monitor plumes from degassing volcanoes that release $SO_2$ into the lower troposphere. Next to total column algorithms, new schemes are becoming mature that provide $SO_2$ plume altitude estimates. The validation of $SO_2$ total column products should cover both eruptive events and degassing cases as well as the layer height, which is most relevant for eruptive cases.

Scenario

- Volcanic eruptive emissions: ground based spectrometers (MAX-DOAS or sun photometers) could be placed near volcanoes that are active over a longer period and for which the chance of capturing the plume is reasonably high. Dedicated and expensive activities are only feasible if the event is large and long lasting.

- Volcanic degassing: long-term observations of $SO_2$ emissions from ground-based scanning DOAS systems (NOVAC), which provide hourly $SO_2$ flux values at a large number of active volcanoes.

Correlative data

- $SO_2$ total column from ground based spectrometers (Pandora, MAX-DOAS)
- $SO_2$ vertical profile information, from ground-based multi-axis DOAS
- $SO_2$ flux measurements from the NOVAC network

Auxiliary data

- Surface reflectance
- Cloud data
- Aerosol data
- Wind information for flux estimates

### 4.1.7. Aerosol Optical Depth

The aerosol amount and microphysical parameters that are by-products or for which assumptions are made in the retrieval need to be compared with reference data, e.g. from ground based sun-photometer measurements (AERONET or Pandora). High resolution (preferably 1 km or smaller) cloud information is important for identifying possible sub-pixel cloud contamination which can strongly impact satellite AOD retrievals.

### 4.1.8. Aerosol Layer Height

The missions Sentinel-4, Sentinel-5, and Sentinel-5P provide an Aerosol Layer Height (ALH) product that is retrieved from measurements in the $O_2$-A band. The product is new and less mature as compared to the other products. A validation of this product requires dedicated effort. Vertical profile data from ground based lidars and ceilometers (EARLINET, AD-NET, E-PROFILE) and from spaceborne lidar instruments such as EarthCare (Adlid), Aeolus, or CALIOP provide a good reference. The aerosol amount and microphysical parameters that are by-products or for which assumptions are made in the retrieval need to be compared with reference data, e.g. from ground based sun-photometer measurements (AERONET or Pandora).

### 4.1.9. Emission Source Estimation

The estimation of emissions of primary pollutants is an important application area of the Geo-AQ missions. It is expected that emissions of $NO_2$ and $SO_2$ are estimated using inverse modelling techniques. Also emissions of Volatile Organic Compounds (methane and non-methane VOC) are expected to be constrained using the observations of HCHO and CHOCHO which are indicators for VOC oxidation. Such estimates will be compared and possibly be used to update existing emission inventories.

An attempt should be made to validate this capability. Satellite observations of known isolated sources should be analysed. Satellite based emission estimates can be compared to the prior knowledge of the source and to estimates made using other methods. Ground based observations of the column density together with wind information on the boundary around the source can be used to estimate the flux across the boundary and the source strength within this boundary. Aircraft imaging spectrometers can provide reference data for the spatial gradients measured by the satellite. Also, reference emission estimates can be made based on such aircraft data.

#### 4.1.10. Recurrent Instruments

For missions with recurrent instruments, tandem operation of the satellite instrument and its successor over at least 1 year should be completed to cover, e.g., a complete annual cycle of the measurand, of its influence quantities and of instrumental properties.

## 4.2. Recommendations for Activities Addressing New Geo-AQ Challenges and Inter-mission Consistency

### 4.2.1. Diurnal Cycle Observation Capability

The sampling of the diurnal cycle of atmospheric constituents is a key feature of the geostationary AQ missions and is new with respect to heritage LEO missions. Temporally varying biases caused by instrument errors (e.g. spectral or radiometric) or by shortcomings in the retrieval (e.g. regarding the treatment of the vertical trace gas profiles, scattering by aerosols and clouds, the surface reflectance and its directionality) may interfere with true diurnal variations. The capability to observe the diurnal cycle needs to be validated.

The validation of this capability is challenging. A combination of airborne, ground-based and in-situ reference measurements is needed to characterise the true diurnal variation accurately and to handle mismatches in representativity between satellite observations and reference measurements. A comprehensive set of auxiliary data is needed to characterise the scene, including the impact of atmospheric scattering and surface reflectance on the radiation field and its directionality, horizontal heterogeneity, the vertical trace gas profile, etc. Therefore dedicated and intensive validation activities at several supersites with a suite of correlative reference measurements are needed, within each Geo-AQ mission domain, where auxiliary data from a variety of sources is exploited.

The acquisition and interpretation of the comprehensive datasets described here is expected to take a considerable effort. These comprehensive datasets are expected to be valuable also for the validation of the satellite products labelled as auxiliary data in the present context. The validation of these products should be coordinated as far as possible with the validation of the Geo-AQ products, in order to fully exploit the effort spent.

**Recommendation 1: Consistently perform intensive campaigns dedicated to the validation of the capability of the Geo-AQ missions to observe the diurnal cycle of the target species. Such campaigns are conducted at several supersites within each Geo-AQ mission domain where a comprehensive suite of correlative reference measurements is made and a comprehensive set of auxiliary data from a variety of sources is exploited.**

Domain

- Several campaigns at various supersites and seasons are needed, per Geo-AQ mission domain, in order to capture a basic set of conditions including polluted and background conditions, as well as overhead and slant illumination conditions (covering the relevant latitudinal and the seasonal ranges). Ideally also dark and bright surfaces should be covered.

- In each campaign, at least ~30 diurnal cycles need to be sampled by a valid set of satellite observations, reference measurements, and auxiliary data. This is necessary to ensure that the dataset captures the day-to-day variation of conditions (local emission characteristics, meteorology, and photochemical regimes, aerosol load, etc.) in a statistically meaningful way. This is also needed to allow the mitigation of possibly large random errors in satellite and reference measurements of HCHO, CHOCHO, and $SO_2$, by data aggregation.
- Airborne measurements characterizing the horizontal and vertical distribution of target species and potential directional biases are expensive. Such measurements might need to be limited to a part of the total campaign, but need to sample multiple days with a complete diurnal cycle, ideally covering various conditions with different local emission characteristics, meteorology, and photochemical conditions. Such measurements are particularly important for $NO_2$ since a) it is a key air quality species with a pronounced diurnal cycle and b) the $NO_2$ satellite product is expected to be susceptible to diurnal retrieval biases, in particular for polluted conditions when mixing ratios peak near the surface.
- The validation data set should include cases that are as simple as possible. The radiation field and its directionality can be best characterised in cases with clear sky conditions, a very low aerosol load, and a Lambertian surface. The diurnal evolution of the pollutants (sources, sinks, photochemical processes, transport) can be best understood in cases with limited transport into the domain.

Correlative measurements

- Total columns of $O_3$, $NO_2$, $SO_2$, and HCHO from ground based spectrometer measurements with high frequency (1-5 minutes) sampling at selected locations (e.g. near the well-characterised sources and at reference background locations).
- Surface concentrations of $O_3$, $NO_2$, HCHO from in-situ sensors measured with high frequency (1-5 minutes) at selected locations (e.g. near the well-characterised sources and at reference background locations).
- Vertical profiles of $O_3$ and $NO_2$ from lidar or balloon borne in-situ measurements, with hourly or better temporal sampling at selected locations (e.g. near the sources and at reference background locations). Profile measurements for $O_3$ need to resolve the free troposphere (for the $O_3$ products of all Geo-AQ missions) and also the near surface concentrations (for the $O_3$ products of TEMPO), in line with the respective retrieval sensitivities.
- Vertical profile information for $O_3$ and $NO_2$ from all-sky mode ground based spectrometer measurements (e.g. Pandora). Such measurement can provide up to 2-3 pieces of information for tropospheric $NO_2$ and a tropospheric sub-column for $O_3$.
- Vertical mixing depth or planetary boundary layer depth with hourly or better temporal sampling, preferably obtained from instruments (e.g., ceilometer, SODAR) co-located with the correlative measurements.
- Local-region tropospheric column data with hourly or better temporal sampling and with high spatial resolution (~1 km) from airborne near-nadir imager spectrometers;

- Multi-directional $NO_2$ tropospheric column data with a variety of illumination and viewing geometries from airborne spectrometers.
- Aerosol amount, absorption, and particle size information, e.g. from ground based sun-photometer measurements.
- Aerosol vertical distribution data from ground based lidar measurements.

Auxiliary data

- Atmospheric chemistry-transport model data that describe the diurnal evolution of sources, sinks, photochemical processes, and spatial distribution (especially the tropospheric profiles) of $NO_2$ and related species (including $NO_x$, OH, and $O_3$).
- 1D photochemical box model describing accurately the diurnal evolution of the $NO_2$ profile and related species in the stratosphere, ideally initiated with atmospheric fields from a 3D/4D chemistry-transport model.
- Estimates of the emission strength of NO and $NO_2$, resolving its diurnal variation
- Surface reflectance directionality (e.g., BRDF) measurements or climatology (monthly resolved map)
- Cloud fraction, optical depth, and height data from meteorological imagers, ground based ceilometers, ground based radars and ground based lidar instruments.
- Multispectral imagers on geostationary satellites (such as the Advanced Baseline Imager (ABI) on GOES-R, the Advanced Meteorological Imager (AMI) on GEO-KOMPSAT-2, or the Flexible Combined Imager (FCI) on MTG-I) bring key information on cloud, aerosol, and surface conditions and on scene heterogeneity.
- Multi-view, multispectral, polarimetric imager data (from LEO sensors such as the Multi-viewing, -channel, -polarisation Imager (3MI) on MetOp-SG, the Directional Polarization Camera (DPC) on GaoFen-5, or the Multi-view Aerosol Mapper (MAP) on the Copernicus candidate mission for anthropogenic $CO_2$ monitoring (CO2M)) offer unique capabilities to distinguish the signatures of surface and aerosol, and hence help to characterise the radiation field and the dependence of the trace gas retrieval sensitivity on the sun-satellite geometry.
- Stratospheric $NO_2$ and $O_3$ data from forecast or (re-)analysis of assimilation systems that take observations as input. Direct observations from ground based passive (e.g. Pandora/FTIR) or active (lidar) are also taken, when available.

### 4.2.2. Airborne and Mobile Ground-based Sensors as Travelling Standards

The exchange of well calibrated reference airborne and ground-based instruments is an essential means to verify consistency of measurements of the Geo-AQ missions. The value of coordinated or joint campaigns with exchange of instrumentation has been demonstrated by the KORUS-AQ and DISCOVER-AQ campaigns. Testing and inter-comparison of airborne $NO_2$ imaging sensors as performed in campaigns such as AROMAT, AROMAT-II, and AROMAPEX is an important step in preparing for the validation of $NO_2$ products and their consistency. Dedicated inter-calibration campaigns (such as the CINDI campaigns for max-DOAS instrumentation) are a prerequisite to establish consistency between the ground-based instrumentation.

**Recommendation 2: Conduct joint validation campaigns with exchange of reference airborne and ground-based instruments.**

### 4.2.3. Inter-mission Radiometric Consistency

The radiometric consistency of the L1b solar irradiance and Earth radiance products and also reflectance derived from these products needs to be assessed systematically and enhanced as far as possible. For the solar irradiance this can be achieved following well established approaches, which are not further discussed here. For the Earth radiance and reflectance this is more complex as one has to deal with the non-overlapping fields of view of the Geo-AQ missions.

One approach is based on the comparison of data acquired over known targets such as very bright clouds and dark ocean scenes. Another is to use SI-traceable data provided by calibration sites under CEOS WGCV umbrella (e.g. RadCalNet and the CEOS WGCV test sites). Statistical analyses of a large collection of measurements with a variety of sun-satellite geometries and conditions are needed to isolate instrument effects. This approach has the potential to verify the radiometric consistency between the missions at minimum and maximum signal levels.

Another approach is based on GEO-LEO collocated measurements and can be applied to a wider range of target scenes. Precise and approximate ray matching techniques as explored by Doelling et al. 2013 (RD22), can be applied to the sub-set of data with comparable sun-satellite geometries. Collocated measurements acquired with different viewing geometries are also valuable for this purpose, as long as the scene directionality can be modelled sufficiently accurately. This can be the case for bright clouds and dark ocean scenes or at radiometric calibration sites used for vicarious calibration of spaceborne imagers, relying on accurate knowledge of surface reflectance and its directionality. The characterisation of the bi-lateral consistency of GEO and LEO pairs of missions is an important result in its own right. When this approach is applied to multiple GEO-LEO pairs, using a LEO mission as the travelling standard, the inter-mission consistency of the geostationary missions is characterised indirectly.

Significant discrepancies should be attributed to specific features of the individual missions and mitigated as far as possible. Radiometric inter-calibration factors should be derived in coordination with the WMO GSICS initiative.

**Recommendation 3: Further develop and eventually apply approaches to the radiometric inter-calibration of the Geo-AQ missions, based on comparisons of Earth radiance data acquired over known targets, SI-traceable test sites where available, precise and approximate ray matching between GEO and LEO pairs of missions, and by taking the LEO missions as a travelling standard. These activities should be pursued within the frame of the WMO GSICS initiative.**

### 4.2.4. Inter-mission Consistency of Level-2 Products

The consistency of the L2 products needs to be assessed systematically and enhanced as far as possible.

Global networks of ground based instruments, such as the NDACC network with Brewer, DOAS, Dobson, FTIR and lidar instruments and the Pandonia Global Network (PGN) with Pandora instruments, include sites within the geographic coverage areas of the three Geo-AQ missions and capitalise on traceable inter-instrument calibration. The long-term systematic validation performed for each mission individually (Section 4.1.2) covers the comparison of L2 products with reference data from such ground based networks. Global analyses of these comparisons should be performed to infer the inter-mission consistency of L2 products.

One approach to cross-validate L2 algorithms is to apply them to a common set of L1b data. A number of issues need to be addressed to make the L2 processors developed for one mission fit for ingesting L1b products from another mission. E.g. the handling of the different L1b product formats, the treatment of flags, and approaches to background correction or the use of reference radiance or irradiance spectra might have to be adapted. If such issues can be addressed, the analysis of L2 data thus obtained is valuable for identifying L2 algorithm issues and discrepancies.

The inter-mission consistency of the stratospheric ozone data needs to be verified. To this end, monthly zonal mean values of the stratospheric sub-column from the ozone profile products should be compared (see Kramarova et al. 2017, RD23), with a consistent definition of the tropopause height. Sampling difference effects need to be taken into account (see Coldewey-Egbers et al. 2015, RD24).

The LEO missions are a valuable asset to validate the inter-mission consistency between the Geo-AQ missions. Most L2 products of the Geo-AQ missions are also covered by the LEO missions S5P, S5, OMPS and EMI (see Table 2.2). Amongst these LEO missions, S5P and S5 are considered very valuable in view of their high spatial resolution that matches the resolution of the GEO missions. Operating from different orbits, S5 and S5P will offer co-locations with Geo-AQ in the mid-morning and the early afternoon, respectively. Additionally, for ozone columns and profiles, data from GOME-2 and from thermal infrared sounders (IASI, IASI-NG, CRiS, or AIUS) should be considered. For the aerosol products, data from multi-view imaging polarimeters (3MI, DPC, or MAP) might be the best candidate for providing LEO reference data. When inter-comparing satellite measurements, special care has to be drawn to differences in spatial resolutions, resulting in possible offsets between satellite observations (Hilboll et al. 2013, RD25). For an accurate interpretation of LEO-GEO comparisons of L2 products scene knowledge is crucial. Therefore, LEO-GEO comparisons should be made systematically at all L2 validation sites for which comprehensive auxiliary information on horizontal and vertical distributions of trace gases, aerosol amount and vertical distribution, surface reflectance and cloud conditions is collected (Section 4.1.3 – 4.1.8).

**Recommendation 4: Further develop and eventually apply approaches to the inter-calibration of the Level-2 products of the Geo-AQ missions. These approaches include the comparison of products with inter-calibrated ground-based network data, cross-validation of Level-2 algorithms by exchanging Level-1b data, comparing zonal mean values of the stratospheric sub-column in the Level-2 ozone products, and taking the LEO missions as a travelling standard.**

### 4.2.5. Level-2 Constellation Products

A common set of L2 algorithms should be agreed for the L2 Constellation Products identified in Section 3.1 ($O_3$ total column, $NO_2$ total column, $NO_2$ tropospheric column, $SO_2$ total column, HCHO total column, CHOCHO total column). A number of issues need to be addressed to make the L2 processors developed for one mission fit for ingesting L1b products from another mission (see previous section).

This set of common L2 algorithms should be used to process L1b data from the various missions, ideally also from one or more of the LEO missions. The systematic generation of L2 Constellation Products generated using the agreed common set of algorithms should be considered.

The analysis of the L2 data thus obtained is expected to be valuable to identify possible L1b issues related to instrument, calibration and processing. Direct comparisons of L2 data from co-located LEO and GEO observations are expected to be meaningful, even when the viewing geometries differ, since L2 processing ideally removes viewing angle dependencies.

**Recommendation 5: Systematically process the Level-2 Constellation Products of the Geo-AQ missions, using one selected common algorithm per Constellation Product.**

## 4.3. Coordination and Continuity

Best practices have been formulated for the quality assurance of the satellite products aiming at the end-to-end traceability of the data quality (see QA4EO framework and e.g. QA4ECV Quality Assurance system). A set of standard reference data has been identified for systematic long-term validation (Fiducial Reference Measurements and other validation data, see Section 1.1 and Table 4.1). The validation activities described in the Sections 4.1 and 4.2 build on a variety of reference data with, to a certain degree, different measurement protocols, QA protocols, data formats, and data policy. It is recommended to make an effort to harmonize also these reference data as far as possible.

**Recommendation 6: Further pursue the harmonization of the reference data used for validation and inter-mission consistency verification of Level-2 products, aiming at common measurement protocols, common QA protocols, common data formats, harmonized data policy and open access.**

Structural funding for all necessary validation/monitoring activities throughout the mission phases, including both long-term systematic and campaign activities, should be maintained. Support for these activities should include a sustainable validation infrastructure including centralised validation facilities (automated as far as possible) and a coordinated pool of experts.

The validation of satellite products and their inter-mission consistency is an effort that relies on the work of many independent groups using a variety of approaches. The validation teams in Asia, Europe, and the US need access to all validation data, including metadata, very soon after acquisition, in order to perform the validation work timely and efficiently. To this end, at least one common and openly accessible data centre needs to be identified for storage and exchange of validation data for the Geo-AQ missions.

**Recommendation 7: Implement a data centre for storage and exchange of all validation data collected for the Geo-AQ missions. Make these data accessible to the entire community involved in the validation of the Geo-AQ mission products and their inter-mission consistency, very soon after acquisition.**

Since the many independent validation groups use a variety of approaches an effort needs to be made to ensure that their validation methods and tools are traceable, mutually consistent, and produce comparable validation metrics and results, across the constellation.

**Recommendation 8: Implement a coordinating unit for ensuring the consistency of the approach and the metrics used for validating the Geo-AQ mission products and their inter-mission consistency.**

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## List of Acronyms

| | |
|---|---|
| AAI | Absorbing Aerosol Index |
| ABI | Advanced Baseline Imager |
| ACC | Atmospheric Composition Constellation |
| AC-VC | Atmospheric Composition Virtual Constellation |
| AD-NET | Asian Dust and Aerosol Lidar Observation Network |
| AERONET | AErosol RObotic NETwork |
| AIUS | Atmospheric Infrared Ultraspectral |
| AMI | Advanced Meteorological Imager |
| AO | Announcement of Opportunity |
| AOD | Aerosol Optical Depth |
| AQ | Air Quality |
| AROMAT | Airborne ROmanian Measurements of Aerosols and Trace gases |
| BRDF | Bi-Directional Reflectance Distribution Function |
| C3S | Copernicus Climate Change Service |
| CAMS | Copernicus Atmosphere Monitoring Service |
| CDR | Critical Design Review |
| CEOS | Committee on Earth Observation Satellites |
| CINDI | Cabauw Intercomparison of Nitrogen Dioxide Measuring Instruments |
| CO2M | Copernicus mission for anthropogenic CO2 Monitoring |
| CrIS | Cross-track Infrared Sounder |
| CLOUDNET | Cloud remote sensing Network |
| CLRTAP | Convention on Long-range Transboundary Air Pollution |
| DISCOVER-AQ | Deriving Information on Surface Conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality |
| DPC | Directional Polarization Camera |
| DOAS | Differential Optical Absorption Spectroscopy |
| EARLINET | European Aerosol Research Lidar Network |
| EC | European Commission |
| EMEP | European Monitoring and Evaluation Programme |
| EMI | Environment Monitoring Instrument |
| ESA | European Space Agency |
| EUMETNET | European Meteorological Services Network |
| E-PROFILE | EUMETNET Profiling Programme |
| FCI | Flexible Combined Imager |
| FRM | Fiducial Reference Measurements |
| FTIR | Fourier Transform InfraRed Spectrometer |
| GAW | Global Atmosphere Watch |
| GCAS | GEO-CAPE Airborne Simulator |
| GEMS | Geostationary Environment Monitoring Spectrometer |
| Geo-AQ | GEOstationary Air Quality Constellation |
| GEO-CAPE | GEOstationary Coastal and Air Pollution Events |
| GeoTASO project | Geostationary Trace gas and Aerosol Sensor Optimization, airborne spectrometer |
| GMES | Global Monitoring for Environment and Security |
| GOCI-2 | Geostationary Ocean Colour Imager |

| | |
|---|---|
| GOES-R/S | Geostationary Operational Environmental Satellite R/S |
| GOME | Global Ozone Monitoring Experiment |
| $GO_3OS$ | Global Ozone Observing System |
| GOSAT | Greenhouse Gases Observing Satellite |
| GSICS | Global Space-based Inter-Calibration System |
| HALO | High Altitude and Long Range Research Aircraft |
| IAGOS | In-service Aircraft for a Global Observing System |
| IASB-BIRA | Royal 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 |
| KORUS-AQ | KORea-United States Air Quality (an international cooperative air quality field study in Korea) |
| LEO | Low Earth Orbit |
| LI | Lightning Imager |
| MAP | Multi-view Aerosol Polarimeter |
| MAX-DOAS | Multi-axis Differential Optical Absorption Spectroscopy |
| MetOp-SG | MetOp-Second Generation |
| MLS | Microwave Limb Sounder |
| MPC | Mission Performance Centre |
| MPLNET | Micro-Pulse Lidar Network |
| MTG | Meteosat Third Generation |
| NASA | National Aeronautics and Space Administration |
| NDACC | Network for the Detection of Atmospheric Composition Change |
| NIER | National Institute of Environmental Research |
| NIR | Near InfraRed |
| NOVAC | Network for Observation of Volcanic and Atmospheric Change |
| NPOESS | National Polar-orbiting Operational Environmental Satellite System |
| OCO | Orbiting Carbon Observatory |
| OMI | Ozone Monitoring Instrument |
| OMPS | Ozone Mapping Profiler Suite |
| PGN | Pandonia Global Network |
| PDR | Preliminary Design review |
| PTU | Pressure Temperature hUmidity radiosonde |
| QA4EO | Quality Assurance framework for Earth Observation |
| QA4ECV | Quality Assurance for Essential Climate Variables |
| RT | Radiative Transfer |
| SCIAMACHY | SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY |
| S-NPP | Suomi National Polar-orbiting Partnership |
| SHADOZ | Southern Hemisphere ADditional OZonesondes programme |
| SSA | Single-Scattering Albedo |
| SWIR | Short Wave InfraRed |
| S4 | Sentinel-4 |
| S5 | Sentinel-5 |
| S5P | Sentinel-5 Precursor |
| TCCON | Total Carbon Column Observing Network |
| TEMPO | Tropospheric Emissions: Monitoring of Pollution |

| | |
|---|---|
| TolNET | Tropospheric Ozone Lidar Network |
| TROPOMI | TROPOspheric Monitoring Instrument |
| TIR | Thermal Infrared |
| UAV | Unmanned Aerial Vehicle |
| UVN | Ultraviolet + Visible + Near infrared |
| UVNS | UVN + Short wave infrared |
| VDAF | Validation Data Analysis Facility |
| VII | Visible/Infrared Imager (MetImage) |
| VIIRS | Visible Infrared Imaging Radiometer Suite |
| WGCV | Working Group on Calibration and Validation |
| WOUDC | World Ozone and Ultraviolet Radiation Data Centre |
| WMO | World Meteorological Organization |
| 3MI | Multi-viewing, -channel, -polarisation Imager |

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# ANNEX: 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

The instrumentation listed below can be mounted on aircrafts or, for light sensors, also on Unmanned Aerial Vehicles (UAV).

- imaging spectrometers (e.g. APEX Airborne PRISM Experiment, AirMAP, SpectroLITE, Small Whiskbroom Imager for trace gases monitoriNG (SWING), GeoTASO and GCAS airborne spectrometers),
- in-situ sensors: electrochemical sensors ($O_3$), chemo-luminiscence based sensors ($NO_2$), laser-induced fluorescence based sensors (various trace gases, including HCHO and $SO_2$), mass spectrometers (all relevant chemical species), nephelometers and particle counters (aerosol).
- (max-)DOAS UV-visible spectrometer: $NO_2$ tropospheric column and profile, also $SO_2$, HCHO, BrO, $O_3$, CHOCHO, possibly aerosols.

### A.1.2 Balloon-borne Instrumentation

- Electrochemical ozonesondes (ECC preferred where available): tropospheric and stratospheric (up to about 30 km) vertical profile of $O_3$ partial pressure, convertible to $O_3$ number density using on-board PTU radiosonde measurements of temperature and water vapour,
- PTU radiosonde (various): tropospheric and stratospheric (up to about 30 km) vertical profile of temperature and water vapour,
- $NO_2$ sonde (equipped with a chemo-luminiscence based sensor).

### A.1.3 Ground-based Instrumentation

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

- Multi-axis DOAS UV-visible spectrometer (M): $NO_2$ tropospheric column and profile, also $SO_2$, HCHO, BrO, $O_3$, CHOCHO, possibly aerosols,
- Zenith-sky DOAS UV-visible spectrometer: stratospheric $NO_2$ and BrO column, $O_3$ total column,
- Direct Sun UV-visible spectrometer (M): $O_3$, $NO_2$, $SO_2$, HCHO total column,
- Direct Sun and almucantar UV-visible spectrometer: $O_3$, $NO_2$, $SO_2$, HCHO total column,
- FTIR spectrometer: column/profile of $O_3$, CO, $CH_4$, water vapour, also $NO_2$ and HCHO,
- Pandora: a spectrometer that can measure in direct sun, direct moon, and sky observation mode (including almucantar, ZS-DOAS, MAX-DOAS etc.). Currently products include vertical columns of $O_3$, $SO_2$, and $NO_2$, and effective $O_3$ temperature. Additional products are in development (HCHO) or planned ($H_2O$, AOD). There is also potential for CHOCHO.
- Brewer and Dobson UV spectrophotometers (double-monochromator Brewers type Mark-IV preferred where available): $O_3$ total column,
- Stratospheric DIfferential Absorption Lidar (DIAL): $O_3$ stratospheric profile,
- Tropospheric DIAL: $O_3$ and water vapour tropospheric profile,
- Tropospheric Raman lidar: water vapour tropospheric profile,
- Aerosol backscatter lidar,
- Aerosol sunphotometer (e.g. Cimel instruments from AERONET),
- Radar/lidar systems measuring cloud properties (e.g. CLOUDNET network),

- Lidars/ceilometers measuring aerosol profile and layer height (e.g. E-PROFILE network),
- In-situ monitoring (regulatory networks, research sites, long-term sites e.g. GAW): $O_3$, $NO_2$, HCHO

## A.2 Monitoring Networks

| Acronym | Infrastructure / Resource | Website / Reference |
|---|---|---|
| AD-NET | AD-Net is a ground-based lidar network for continuous observation of vertical distributions of aerosol and cloud in East Asia. AD-Net is also a contributing network to the GAW Aerosol Lidar Observation Network (GALION) | http://www-lidar.nies.go.jp/AD-Net/ |
| AERONET | AErosol RObotic NETwork: global network of inter-calibrated multispectral sun-photometers measuring aerosol optical depth and several other aerosol characteristics. | https://aeronet.gsfc.nasa.gov |
| CEOS calibration test sites | Test sites studied and selected by CEOS WGCV that can be used for the calibration and characterisation of different sensor type | http://calvalportal.ceos.org/calibration-test-sites |
| CLOUDNET | Cloudnet remote sensing network measuring vertical profiles of cloud and aerosol properties at high temporal and spatial resolution in Europe | http://www.cloud-net.org |
| EARLINET | European Aerosol Research Lidar Network: European network of ground-based lidar instruments for profiling of aerosol and clouds. | https://www.earlinet.org |
| EMEP | Co-operative European Monitoring and Evaluation Programme (EMEP) for the Long-range Transmission of Air Pollutants in Europe. Surface monitoring of $O_3$, $NO_2$, $SO_2$, particles (PM)… | http://www.emep.int |
| EUMETNET | European Meteorological Services Network (EUMETNET) E-PROFILE: Profiling Programme providing wind observations from weather radars and dedicated wind profilers and Lidar/Ceilometer observations | http://eumetnet.eu |
| IAGOS | In-service Aircraft for a Global Observing System: European Research Infrastructure for global observations of atmospheric composition from commercial aircraft. In-situ sensors on measuring along-route $O_3$, CO, $CO_2$, $CH_4$, $NO_x$, $NO_y$, $H_2O$, aerosols and cloud particles. Successor of MOZAIC programme. | https://www.iagos.org |

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| GAW | World Meteorological Organization's Global Atmosphere Watch programme: in-situ monitoring networks and contributing networks like NDACC, SHADOZ and TCCON. | http://www.wmo.int/pages/prog/arep/gaw/gaw_home_en.html |
| MPLNET | NASA's Micro-Pulse Lidar Network: a federated network of lidar systems designed to measure aerosol and cloud vertical structure, and boundary layer heights. Most MPLNET sites are co-located with AERONET sites. MPLNET is also a contributing network to the GAW Aerosol Lidar Observation Network (GALION). | https://mplnet.gsfc.nasa.gov/ |
| NDACC | Network for the Detection of Atmospheric Composition Change: global network of remote sounding research stations with a variety of instruments: Brewer and Dobson spectrophotometers ($O_3$), DOAS UV-Visible spectrometers (Zenith-sky: $O_3$, $NO_2$, BrO, OClO; Multi-axis: $NO_2$, HCHO, $SO_2$…), FTIR spectrometers ($CH_4$, CO, $N_2O$, CFCs, $H_2O$…), lidars (stratospheric and tropospheric $O_3$, $H_2O$, temperature, aerosols), millimeter wave radiometers ($O_3$, $H_2O$, ClO), UV spectral irradiance instruments, ozone sondes, and aerosol backscatter sondes. | http://ndacc.org |
| NOVAC | Network for Observation of Volcanic and Atmospheric Change (NOVAC): community of volcano observatories and research institutions that together develop and apply ultraviolet differential optical absorption spectroscopy (DOAS) instruments to measure volcanic gas emission rates. | http://novac-community.org |
| PGN | Pandonia Global Network: Network of inter-calibrated Pandora instruments (UV-vis spectrometers) measuring a variety of species ($O_3$, $SO_2$, $NO_2$, …); currently growing into a global network. | http://pandonia.net<br>http://pandonia-global-network.org |
| RadCalNet | RadCalNet provides SI-traceable Top-of-Atmosphere (TOA) spectrally-resolved reflectances to aid in the post-launch radiometric calibration and validation of optical imaging sensor data: continuously updated archive of TOA reflectances derived over a network of sites, with associated uncertainties, at a 10 nm spectral sampling interval, in the spectral range from 380 nm to 2500 nm and at 30 minute intervals. | https://www.radcalnet.org |

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|---|---|---|
| SHADOZ | NASA's Southern Hemisphere ADditional Ozonesondes programme: ozonesonde stations operating in the tropics, subtropics, and in the southern hemisphere in general, with coordinated launches and a central archive. Network operating since 1998. | https://tropo.gsfc.nasa.gov/shadoz |
| TCCON | Total Carbon Column Observing Network: global network of Fourier Transform near-infrared Spectrometers recording direct solar spectra for the measurement of atmospheric $CO_2$, $CH_4$, $N_2O$, HF, CO, $H_2O$, and HDO. | http://tccon.caltech.edu/ |
| TOLNet | Tropospheric Ozone Lidar Network: North-American network of ground-based lidar instruments for profiling of tropospheric ozone. | https://www-air.larc.nasa.gov/missions/TOLNet |
| $GO_3OS$ / WOUDC | WMO's Global Ozone Observing System / World Ozone and Ultraviolet Radiation Data Centre: centrally archived global network of total ozone column instruments: Brewer and Dobson spectrophotometers, ozonesondes, Russian UV filter radiometers, stratospheric ozone lidars, Umkehr $O_3$ profiling, UV-visible DOAS spectrometers. | http://woudc.org |

## A.3 Cal/Val Data Archives, Validation Servers, and Other Resources

| Name | Infrastructure / Resource | Website / Reference |
|---|---|---|
| ACTRIS | European Research Infrastructure for the observation of Aerosol, Clouds, and Trace Gases (ACTRIS) | http://www.actris.eu |
| AVDC | Aura Validation Data Center (AVDC, at NASA-GSFC) in support of EOS-Aura and other A-Train validation and science activities | https://avdc.gsfc.nasa.gov |
| CEOS Cal/Val | CEOS Cal/Val Portal: various Cal/Val tools, methods and data for the EO community | http://calvalportal.ceos.org |
| CAMS-NDACC | Copernicus Atmosphere Monitoring Service automated NDACC-based evaluation system (CAMS-84, at IASB-BIRA) | http://nors-server.aeronomie.be |
| EVDC | ESA Validation Data Centre (EVDC, at NILU): Cal/Val data and tools for all ESA EO missions | http://evdc.nilu.no |
| GSICS | WMO-CGMS Global Space-based Inter-Calibration System (GSICS): monitoring and calibration of operational weather and environmental satellites | http://gsics.wmo.int |
| ICARE | Cloud/Aerosol/Water/ Radiation Interactions Thematic Center (at University of Lille): production, comparison and distribution of EO data on aerosols, clouds, radiation and water cycle | http://www.icare.univ-lille1.fr |
| Multi-TASTE | IASB-BIRA Multi-TASTE versatile system for multi-satellite validation, network homogeneity evaluation, and support to algorithm evolution | Keppens et al. 2018 (RD26), Verhoelst et al. 2015 (RD21) |
| NPROVS | NOAA Products Validation System (NPROVS): routine comparison of temperature and water vapour data from satellites, sondes and NWP | https://www.star.nesdis.noaa.gov/smcd/opdb/nprovs/ |
| OSSSMOSE | IASB-BIRA Observing Systems of System Simulator for Multi-mission Synergies Exploration: simulator of real and hypothetical | Verhoelst et al. 2015 (RD21) |

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|---|---|---|
| | observing systems and associated uncertainties with explicit 3D comparison metrology, co-location optimization, and error budget closure | |
| QA4ECV-AVS | QA4ECV Atmosphere Validation Server for ECV Precursors (EC FP7 QA4ECV project): automated comparison of satellite and ground-based ECV data records of $NO_2$, HCHO and CO | https://qa4ecv-dev.stcorp.nl |
| QA4ECV QA System | QA4ECV QA System: resources to generate EO-based ECV products with embedded QA information and to assess their fitness-for-purpose for applications (EC FP7 QA4ECV project) | http://www.qa4ecv.eu/qa-system |
| S5P VDAF | Sentinel-5p MPC validation website and its Validation Data Analysis Facility / Automated Validation Server (VDAF, at IASB-BIRA): automated validation server for TROPOMI Level-2 data products ($O_3$, $NO_2$, HCHO, $SO_2$, CO, $CH_4$, clouds (CF, CTH, COD), aerosols (AAI, ALH) | http://s5p-mpc-vdaf.aeronomie.be/ <br> http://mpc-vdaf-server.tropomi.eu |